

SYMPOSIUM P

Growth, Evolution, and Properties of Surfaces, Thin Films, and Self-Organized Structures

November 27 – December 1, 2000

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* Invited paper

SESSION P1: NANOSCALE SURFACE
STRUCTURES

Chair: Franz J. Himpsel
Monday Morning, November 27, 2000
Room 302 (Hynes)

8:30 AM P1.1

OXIDE NANOSTRUCTURES THROUGH SELF-ASSEMBLY. S. Aggarwal, S.R. Shinde, S.B. Ogale, V.A. Novikov, A.P. Monga, and R. Ramesh Department of Materials and Nuclear Engineering University of Maryland, College Park, MD; V. Ballarotto and E.D. Williams Department of Physics, University of Maryland, College Park, MD.

A prominent theme in inorganic materials research is the creation of UNIFORMLY FLAT thin films and heterostructures over large wafers, which can subsequently be lithographically processed into functional devices. This paper proposes an approach that will lead to thin film topographies that are directly counter to the above-mentioned philosophy. Recent years have witnessed considerable research activity in the area of self-assembly of materials, stimulated by observations of self-organized behavior in biological systems. We have fabricated uniform arrays of NON-PLANAR surface features (which we term "TIPS") by a spontaneous assembly process involving the oxidation of simple metals, especially under constrained conditions on a variety of substrates, including glass and Si. We demonstrate the pervasiveness of this process through examples involving the oxidation of Pd, Cu, Fe and In. We demonstrate that the feature sizes can be controlled through the grain size and thickness of the starting metal thin film. Finally, such sub-micron scale arrays can serve as templates for the design and development of a broad range of self-assembled, nanoelectronic devices. S. Aggarwal et al, Science 287, 2235 (2000)

8:45 AM P1.2

NOVEL AND FLEXIBLE SELF-ORGANIZED ROUTES FOR NANOSCALE PATTERNING. Sebastiaan van Dijken and Bene Poelsema, University of Twente, MESA Research Centre and Faculty of Applied Physics, Enschede, THE NETHERLANDS.

The evolution of the morphology of growing Cu(001) has been studied in detail using HR-LEEM in distinctly different geometries: The molecular beam was either oriented normal to the surface or at glancing incidence. In both cases self-organization during growth leads to novel, previously unanticipated patterns. At normal incidence, quite regular pyramids are formed with step edges along $\langle 110 \rangle$. These pyramids assume a checkerboard like pattern, with well-established short-range order and weak long-range order. After grazing incidence deposition the surface exhibits a distinct two-fold symmetry in contrast to the expected and measured four-fold symmetry at normal incidence. At grazing incidence remarkably well ordered arrays of parallel linear structures emerge. The mechanisms underlying the development of both structures will be discussed in detail. The experiment has disclosed an unanticipated mechanism, i.e. the steering of atoms by long-ranged dispersion forces. This novel feature gives rise to increased kinetic roughening and becomes particularly important during MBE at grazing incidence. Where increased roughness is usually valued negatively, the steering phenomenon can also be made of advantage for the preparation of highly regular arrays of parallel ripples. This feature is highlighted below: Deposition of thermal energy copper atoms at about 80° (from the normal) results in parallel ripples oriented perpendicular to the (MBE-) plane of incidence. The diffraction spot profiles, measured after deposition of several tens of monolayers, show remarkable ordering. They reveal well-developed facets with orientations of corresponding to (111) and (113) on the illuminated and the shadow sides of the ridges, respectively. The distance between the ridges is determined by the adatom mobility. By varying the substrate temperature between about 220 and 350 K their mutual separation changes from about 3 to 25 nm. The obtained results are believed to be of general interest to homo- and heteroepitaxial growth systems.

9:00 AM P1.3

MICROSTRUCTURE DEVELOPMENT IN OBLIQUELY DEPOSITED THIN FILMS. F. Paritosh, University of Michigan, Dept of Chemical Engineering, Ann Arbor, MI; David J. Srolovitz, Dept of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ.

Thin films deposited from a flux that is directed other than normal to the substrate (i.e., oblique deposition) commonly exhibit microstructures characterized by grain structures with boundary and/or voids tilted away from the substrate normal, void incorporation and varying density. This suggests that it is possible to fabricate anisotropic microstructures by varying the deposition angle either spatially or temporally during growth. Spatial variations are common since deposition fluxes are never perfectly collimated. In the present study, we apply a front tracking method to simulate microstructure evolution over a range of oblique deposition

geometries. In order to focus on the fundamental essence of this effect, we have developed a model that incorporates self-shadowing, but excludes other physical effects such as surface diffusion, surface/interfacial energy anisotropy and grain boundary migration. Our simulations predict the temporal evolution of the microstructure, morphology and texture of the polycrystalline film. We present the results of the evolution of mean grain size and void size, grain size distribution, orientation of void tracks and grain boundaries, and crystallographic texture as a function of deposition angle. As in the experiments, the microstructures produced in this way tilt away from the substrate normal as the deposition flux becomes increasingly oblique. Conditions exist for which this relationship is well described by the classical tangent law. We also demonstrate that crystallographic texture can be modified using oblique deposition. Finally, we examine the effects of the angular dispersion in the deposition flux and time-varying deposition angles on microstructure evolution during film growth.

9:15 AM *P1.4

DIRECT OBSERVATIONS OF SELF-ASSEMBLED DOMAIN STRUCTURES AND THEIR DYNAMICS: Pb ON Cu(111). R. Plass, Sandia National Laboratories, Albuquerque, NM; N.C. Bartelt, Sandia National Laboratories, Livermore, CA; G.L. Kellogg, Sandia National Laboratories, Albuquerque, NM.

The spontaneous formation of self-assembled, two-dimensional domain structures in two-phase systems is of both scientific and technological interest. Theoretical investigations of the stability of periodic structures due to long-range, dipolar interactions predict an interesting progression of droplet and striped phases as a function of area fraction [1]. Experimental verification of the theory, however, has been elusive. Using low energy electron microscopy (LEEM), we find that submonolayer growth of Pb on Cu(111) reproduces the predicted domain evolution with surprising accuracy. Pb on Cu(111) follows the SK growth mode with a disordered surface alloy saturating at 0.4 ML Pb and an incommensurate overlayer covering the surface at 1.0 ML[2]. Our LEEM observations show that during Pb deposition at 385C, droplets of the incommensurate structure (about 90 nm in diameter) grow in the surface alloy matrix with increasing density. The droplets clearly repel each other and pack together into a fairly well-ordered lattice. They achieve maximum density near 0.3 area fraction, after which there is an abrupt transition to a striped phase characterized by lengthening bands of surface alloy and incommensurate regions. The stripes completely cover the surface at 0.5 area fraction, after which another abrupt transition occurs to an inverse droplet phase (surface alloy droplets in the incommensurate matrix). The droplet-stripe-inverse droplet transitions and boundary length as a function of area fraction are all in excellent agreement with theory[1]. The domain structures' spatial dimensions, as well as the size of their thermal fluctuations are temperature sensitive. We use this sensitivity to probe the energetics responsible for the domain structures. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin company, for the U.S. DOE under contract #DE-AC04-94AL85000

[1] K.-O. Ng and D. Vanderbilt, Phys. Rev. B 52 (1995) 2177.

[2] C. Nagl, et al., Surf. Sci. 321 (1994) 237.

10:00 AM *P1.5

DYNAMIC STM STUDIES OF THE NUCLEATION AND GROWTH OF SELF-ORGANISED NANOSTRUCTURES. Flemming Besenbacher, Institute of Physics and Astronomy and Center for Atomic-scale Materials Physics, University of Aarhus, Aarhus, DENMARK.

Scanning tunneling microscopy (STM) has proven to be a fascinating and powerful technique capable of resolving single atoms and molecules on surfaces and revealing the dynamics of surface processes by the recording of many sequential STM images with a fast-scanning, variable-temperature STM [1]. In this talk I will show how STM movies can be used to dynamically follow the nucleation and growth of self-organised nanostructures on surfaces. In the first example we have studied the self-assembly of largish molecules, hexa-tert-butyl decacyclene (HtBDC) on Cu(110) and found that the molecules arrange in a double chain self-assembled structure. By manipulating the individual molecules we have revealed that, surprisingly, the supramolecular aggregation is induced by a restructuring of the topmost surface layers below the self-assembled molecular layer [2]. In the second example we have followed the nucleation and growth of an O-induced nanostructure on Pt(110). Long-range elastic interactions cause this nanostructure to self-organize over mesoscopic length scales into a (11x2) O-nanograting. We will show how this nanopattern can be used as a template to tailor the epitaxial growth metal islands with a narrow size distribution [3].

1. F. Besenbacher, Scanning Tunneling Microscopy studies of metal surfaces, Reports on Progress in Physics 59 (1996) 1737

2. M. Schunack, L. Petersen, A. Kühnle, E. Lægsgaard, I. Stensgaard, I. Johannsen, F. Besenbacher, submitted

3. S. Helveg, S. Horch, E. Lægsgaard, I. Stensgaard, F. Besenbacher, to be published

10:30 AM P1.6

PREFERENTIAL NUCLEATION AND SELF-LIMITING GROWTH OF METAL NANOCLUSTERS ON S(4X4)/W(111). Q. Wu, W.

Chen, T.E. Madey, Dept. of Physics and Astronomy and Laboratory for Surface Modification, Rutgers University, Piscataway, NJ.

Interactions of Cu and Pt with the highly ordered S(4x4)/W(111) surface have been studied by means of Auger electron spectroscopy (AES), low energy electron diffraction (LEED), and scanning tunneling microscopy (STM). The substrate is a sulfur-induced nanoscale reconstruction of W(111) with (4x4) periodicity, characterized by broad, planar terraces (~30 nm in width). We find that fractional monolayers of vapor-deposited Cu grow as clusters on the S(4x4) surface over a wide coverage range. At low Cu coverages (< 0.1 ML), Cu nanoclusters are observed to nucleate preferentially at characteristic 3-fold hollow sites on the S(4x4) surface; there is a clear energetic preference for one type of site over others. The formed Cu nanoclusters are uniform in size (~0.7 nm) up to 0.25 ML, indicating self-limiting growth. As coverage increases, additional sites are populated and Cu clusters grow in size. On the other hand, Pt exhibits a different behavior, disordering the (4x4) reconstruction and adsorbing beneath the outer S-layer. STM data are supported by LEED and AES measurements. The data are interpreted in terms of relative surface free energy, relative reactivity, and the metal-W, metal-S, and S-W binding energies, as supported by our previous TPD data.

10:45 AM P1.7

SELF-ORGANIZED NANOSCALE PATTERN FORMATION ON VICINAL Si(111) SURFACES VIA A TWO-STEP FACETING TRANSITION. F.K. Men, National Chung Cheng University, Dept of Physics, Chia-Yi, Taiwan, ROC; Feng Liu, University of Wisconsin, Dept of MS&E, Madison, WI.

We demonstrate self-organized pattern formation on vicinal Si(111) surfaces that are miscut toward the [-211] direction. All the patterns, consisting of a periodic array of alternating (7x7) reconstructed terraces and step-bunched facets, have the same periodicity and facet structure, independent of the miscut angle; while the width of the facets increases linearly with increasing miscut angle. We attribute such unique pattern formation to a surface faceting transition that involves two transition steps: the first step forms a stress-domain structure defining the universal periodicity; the second step forms the low-energy facets controlling the facet width.

11:00 AM *P1.8

SELF-ORGANIZED GROWTH OF SURFACE SUPPORTED NANOSTRUCTURES. Klaus Kern, Max-Planck-Institut fuer Festkoerperforschung, Stuttgart, GERMANY.

The physical and chemical properties of low-dimensional structures are unique functions of their size and shape and differ largely from the behavior of bulk matter. Particularly fascinating phenomena occur if the nanostructures are subject to lateral boundary conditions on a length scale where quantum behavior prevails; magnetic nanostructures can be made out of traditionally nonmagnetic elements, catalytic activity can emerge from elements as inert as Au and new electronic quantum devices can be built. Much effort has been devoted to create metal and semiconductor nanostructures at surfaces. Their controlled fabrication, in particular the creation of lateral order, however, remains an experimental challenge. In this talk we will focus on the fabrication of nanostructures via self-organized growth at surfaces. Advantages and limitations of diffusion controlled molecular beam epitaxy will be discussed and novel routes for the fabrication of ordered arrays of nanostructures will be presented. By way of illustration the growth of one- and two-dimensional arrays of metal nanostructures, luminescent Ge quantum dots and supramolecular nanogratings will be discussed in detail.

11:30 AM P1.9

TAILORING THE SIZE AND SHAPE OF METALLIC NANOSTRUCTURES THROUGH LASER IRRADIATION DURING AND AFTER GROWTH. Frank Stietz, Johannes Bosbach, Thomas Wenzel, Frank Träger, University of Kassel, Kassel, GERMANY.

Self assembly of metal atoms on dielectric surfaces is a widely used technique to generate nanometer sized metal aggregates. Main reasons are that particles of almost any desired size can be made by variation of the growth conditions and that it is comparably easy to apply. Usually, however, two problems arise. First, broad size distributions are generated which obscure the size dependent characteristics of the nanoparticles. Secondly, simultaneous change of the diameter and the shape of the aggregates occurs, making an independent control of both parameters almost impossible. Here we show that laser

irradiation of metallic nanostructures generated by self assembly of metal atoms on oxide surfaces can be used to overcome these problems. For this purpose, the size and shape dependent optical properties of metal aggregates, i.e. surface plasmon excitation in the particles, and the ability to remove atoms from their surfaces in a controlled manner by laser evaporation are exploited. Irradiation of the samples during growth of the nanostructures allows to fabricate particles with predetermined shape irrespective of the size. The actual shape can be chosen in advance, since it is determined by the laser photon energy. Irradiation after growth can be exploited for considerable narrowing of broad size distributions yielding almost monodispersed samples. The methods are demonstrated experimentally for Ag and Au particles with diameters between 1 and 25 nm on different oxide surfaces including SiO₂ and Al₂O₃. By using nanosecond laser pulses of three different photon energies during growth, oblate particles with three fixed aspect ratios have been fabricated. Applying the laser light after growth results in a narrowing of the size distributions by more than 60% yielding distributions with normalized standard deviations of about 10%. Furthermore, a theoretical model is presented which allows one to describe laser manipulation of metal nanostructures quantitatively.

SESSION P2: PATTERN FORMATION ON SURFACES

Chair: Michael S. Altman

Monday Afternoon, November 27, 2000

Room 302 (Hynes)

1:30 PM *P2.1

NOVEL FORMATION MECHANISMS OF TWO-DIMENSIONAL ISLANDS ON SURFACE IN THE PRESENCE OF ADSORBATES. J. Wu, B.G. Liu and E.G. Wang, Institute of Physics, CAS, Beijing, CHINA; Zhenyu Zhang, Oak Ridge National Laboratory, Oak Ridge, TN.

A rich variety of two-dimensional patterns can be formed in the early stages of film growth. In this talk, we will show that, when a surfactant layer is used to mediate the growth, a counter-intuitive fractal-to-compact island shape transition can be induced by increasing deposition flux or decreasing growth temperature. Specifically, we develop the reaction limited aggregation (RLA) theory, where the essential physical process controlling the island shape transition is the shielding effect of adatoms stuck to stable islands on incoming adatoms.[1] Comparisons with experimental observations will be made.[2] Also discussed are the selection mechanisms of 2D island shapes in the compact regime, as observed, in Pt (111) homoepitaxy without or with the presence of CO as adsorbates.[3,4] We will provide a coherent and unified picture for the interpretation of these intriguing observations based on kinetic Monte Carlo simulations, with energy barriers from first-principles calculations.[5]

[1] B.G. Liu, J. Wu, E.G. Wang and Z. Zhang, Phys. Rev. Lett. 83, 1195 (1999).

[2] T.C. Chang, J.S. Hwang and T.T. Tsong, Phys. Rev. Lett. 83, 1191 (1999).

[3] T. Michely, M. Hohage, M. Bott and G. Comsa, Phys. Rev. Lett. 79, 3943 (1993).

[4] M. Kalff, G. Comsa and T. Michely, Phys. Rev. Lett. 81, 1255 (1998).

[5] J. Wu, E.G. Wang, B.G. Liu and Z. Zhang, Phys. Rev. Lett. (2000, submitted).

2:00 PM P2.2

NANOSCALE PATTERN FORMATION OF AN EPITAXIAL MONOLAYER GROWN ON A SOLID SURFACE. W. Lu and Z. Suo, Mechanical and Aerospace Engineering Department and Princeton Materials Institute, Princeton University, Princeton, NJ.

A two-phase epilayer on an elastic substrate may form stripes or dots on the scale of nanometers. Sometimes these stripes and dots may self-organize into superlattices. This paper reports on a simulation of the pattern formation process. We show that the size selection and self-organization can both result from two competing actions: the phase boundary energy tends to coarsen the phases, and the concentration-dependent surface stress tends to refine the phases. A nonlinear diffusion equation couples the concentration field in the epilayer and the stress field in the substrate. The simulation reveals rich dynamics. An epilayer may evolve into various patterns, suggesting a significant degree of experimental control in growing nanoscale superlattices. For further information, see our web page: www.princeton.edu/~suo.

2:15 PM P2.3

HIGH RESOLUTION TEM STUDIES OF 3D GOLD ASSEMBLED PARTICLES. Miguel José Yacamán, Instituto de Física, UNAM and

Instituto Nacional de Investigaciones Nucleares; C. Gutiérrez-Wing, J.A. Ascencio, M. Pérez and A. Camacho, Instituto Nacional de Investigaciones Nucleares, MEXICO.

Self assembled superlattices of gold nanoparticles are studied using high resolution TEM and high dispersion diffraction methods. The optimal objective lens focusing condition for observation of the superlattice is discussed. It is found that by controlling the particle size and the crystallization condition it is possible to produce different crystalline structures such as cubic or hexagonal close packing or tetragonally distorted FCC. The conditions in which each structure is produced is discussed. The evolution of the superlattice of the self assembled nanoparticles with temperature is also reported. The studies were carried out by in situ heating in the high resolution TEM. The temperatures were varied until reaching the melting point of the superlattice. The melting mechanism is discussed.

3:00 PM *P2.4

SELF-ORGANIZED ARRAYS OF DOTS AND STRIPES AT STEPPED SURFACES. Franz J. Himpel, Univ Wisconsin Madison, Dept of Physics, Madison, WI.

Self-organized nanostructures are an ideal testbed for preparing tailored solids, whose electronic properties are controlled by confinement or by proximity to interfaces. Here we explore one- and zero-dimensional structures, such as arrays of stripes and strings of dots. Stepped surfaces serve as templates for self-organization. Some of the techniques of microlithography can be extended to the nano-regime, such as the use of an inert mask and the selective deposition between the masked areas. Examples from a variety of applications will illustrate the process [1]: • The preparation of step arrays on silicon with kink densities as low as one in 20,000 and step spacings controllable from 2 to 80 nm. • The epitaxial growth of calcium fluoride masks, either as stripes or as strings of dots. • A new growth mode on stepped Si(111) that replaces stripe flow and produces linear dot arrays with a density of 2 Teradots per square inch. [2] • Selective adsorption of molecules between calcium fluoride stripes and its extension to selective CVD of iron nanowires. • Organic molecules and DNA snippets on stepped silicon structures that are made bio-compatible via thiol-gold chemistry. • One-dimensional chains of gold on stepped Si(111) with exotic band structures. [3]

[1] F.J. Himpel, T. Jung, A. Kirakosian, J.-L. Lin, D. Y. Petrovykh, H. Rauscher, and J. Viernow, *MRS Bulletin* 24 (8), 20 (1999).

[2] Adam Li, Feng Liu, D.Y. Petrovykh, J.-L. Lin, J. Viernow, F.J. Himpel, and M.G. Lagally, to be published.

[3] R. Losio, K. N. Altmann, and F. J. Himpel, *Phys. Rev. Lett.*, in press.

3:30 PM P2.5

DIFFUSION, NUCLEATION AND GROWTH ON PATTERNED SUBSTRATES. J.A. Venables, Arizona State University, Dept of Physics & Astronomy, Tempe, AZ and University of Sussex, CPES, Brighton, UNITED KINGDOM.

Nucleation and growth models are well developed for nucleation on homogeneous substrates, and can typically be described in terms of three energy parameters. A few cases of nucleation on substrates containing defect traps have been investigated, at the cost of introducing (at least two) more parameters. Growth methods using patterned substrates and/or self-organization may offer technological advantages, but they also pose some scientific challenges. One of these is to define a suitably small set of geometries and energy regimes, which can then be analyzed in closed form. A dimensional classification is attempted, and some examples are related to recent experiments, using rate and rate-diffusion equations. Caution is needed, since most relevant energies are composite, and models may have a many-to-one relationship to experiment.

3:45 PM P2.6

DYNAMICS OF InAs QUANTUM DOTS FORMATION ON AIAs AND GaAs. M. Yakimov, V. Tokranov, and S. Oktyabrsky, Center for Advanced Thin Film Technology, University at Albany - SUNY, Albany, NY.

We have studied the formation of InAs quantum dots (QDs) grown by molecular beam epitaxy on top of GaAs and 2 ML-thick AIAs overlayers in a temperature range from 400°C to 500°C. In-situ reflection high energy electron diffraction (RHEED) patterns were recorded in real time during the growth and analyzed to reveal the moment of 2D-3D transition in RHEED pattern, indicating the QD formation, ripening process and subsequent overgrowth. The kinetics of QD formation was studied using In fluxes corresponding to the growth rate of InAs ranging from 0.01 to 1 ML/s at different As₂ pressures. Evolution of the RHEED patterns was analyzed also to reveal the development of sizes and shapes of the QD ensemble. The critical InAs coverage for QD formation was shown to be 15% higher (at 400°C) for dots grown on the AIAs overlayer than for those grown

on the top of GaAs. The critical coverage increases for temperatures above 475°C for both materials. At lower temperatures, the critical coverage is almost independent of temperature for GaAs, but exhibits a distinct minimum at 450°C if grown on AIAs overlayer. The increase of the critical coverage with temperature reduction is attributed to the lower surface diffusion rates of adatoms on the AIAs surface.

4:00 PM P2.7

SELF-ORGANIZED COARSENING OF TWO-DIMENSIONAL ISLANDS VIA STRAIN-DIRECTED ISLAND MOTION. Feng Liu, Adam H. Li, and M.G. Lagally, University of Wisconsin, Dept of MS&E, Madison, WI.

We show that in coarsening of two-dimensional islands, the strain-induced island-island interaction not only modifies the average chemical potential of islands but also produces a chemical-potential gradient within each island. Computer simulations show that the chemical-potential gradient causes effectively a strain-directed island motion in systems where island edge diffusion is significant, which leads to self-organization of a triangular lattice of island arrays with uniform size and spacing.

4:15 PM P2.8

PERIODICAL DISLOCATION NETWORKS OF Ge FILMS ON Si(111). Th. Schmidt, J. Falta, Univ Bremen, Bremen, GERMANY; P. Zahl, M. Kammmer, P. Kury, Univ Hannover, Hannover, GERMANY; M. Horn-von Hoegen, Univ Essen, Essen, GERMANY.

Thin Ge films grown on Si(111) have been investigated by spot profile analysis low energy electron diffraction (SPA-LEED) and grazing incidence x-ray diffraction (GIXRD). At a substrate temperature of about 700°C, Ge films were grown by Sb surfactant mediated epitaxy (SME). Using this growth technique, 3D island formation can be suppressed, which is always observed in conventional molecular beam epitaxy (MBE). Deposition on Si(111) in contrast to Si(001) allows the growth of defect-free Ge films. This is accomplished by the formation of a dislocation network confined to the Ge/Si interface. The present work focuses on GIXRD experiments performed on such misfit dislocation networks. Reciprocal space maps have been recorded in the vicinity of different in-plane as well as out-of-plane Bragg spots. Additional satellite spots are observed which reflect the periodical distortion of the crystal lattice due to the periodical arrangement of interfacial dislocations. From the satellite peak position and separation, the Ge lattice constant and the average distance between adjacent dislocations can be determined. From our data, we find that the residual strain within Ge films of 50 Å thickness is about 1.0% and decreases with increasing film thickness. From an analysis of the width and the relative integral intensity of the satellite spots (as a function of momentum transfer), information can be obtained concerning the ordering of the dislocation network. By comparison to simulations, the GIXRD may also be used to determine the dislocation structure.

4:30 PM *P2.9

SHEDDING LIGHT ON SURFACE REACTIONS: IMAGING PATTERN FORMATION FROM ULTRA-HIGH VACUUM UP TO HIGH PRESSURES. Harm Hinrich Rotermund, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Dept. of Physical Chemistry, Berlin, GERMANY.

This talk focuses on imaging of dynamic processes on surfaces, using light to illuminate the area of interest. The main emphasis will be on pattern formation during CO-oxidation on Pt surfaces. The most recent techniques, mainly Ellipso-Microscopy for Surface Imaging (EMSI), based on an ellipsometric effect, and Reflection Anisotropy Microscopy (RAM) using different reflectivity properties of non-isotropic surfaces, expand the range of observable pressure conditions formerly accessible by the Photoemission Electron Microscope (PEEM) by many orders of magnitude, thus bridging the pressure gap in imaging surface reactions. An advanced version of the RAM, using just white light and a combination of lenses with a Foster-prism, allows now the observation of macroscopic pattern formation during heterogeneous reactions with their submonolayer coverages by eye alone. The underlying contrast mechanism of EMSI and RAM will be discussed. For a certain range of the control parameters, which are the partial pressures of the reactants and the temperature of the sample, self organization in form of pattern formation like spiral waves, target patterns, solitary waves and standing waves including chaotic behavior can be observed. A short video will demonstrate the great richness of spatio-temporal pattern formation during surface reactions under partial pressures below 0.001 mbar up to the 1000 mbar region.

SESSION P3: POSTER SESSION
SURFACE DIFFUSION AND GROWTH, MAGNETIC
FILMS, AND NANOSTRUCTURES ON SURFACES

Chair: Theodore E. Madey
Monday Evening, November 27, 2000
8:00 PM
Exhibition Hall D (Hynes)

P3.1

**SURFACE SELF-DIFFUSION INSTABILITY IN ELECTRIC
FIELDS.** Michael I. Ojovan, Pavel P. Poluectov, Scientific and
Industrial Association "Radon", Moscow, RUSSIA.

The plane form is equilibrium one for surfaces of condensed matter. Deviations can be caused usually by crystal structure. Herein we will describe an effect of surface instability due to self-diffusion processes of atoms and molecules in the near surface electric field. Self-diffusion processes (as it was shown by Mullins) cause relaxation of any deviation (protuberance) from the plane form due to the increased concentration of surface atoms and its consequent smoothing. This process we studied for the case when there is an electric field near the surface. The near surface electric field can be due to either the location of material in an external (homogeneous or inhomogeneous) electrical field or self-charges on the surface. There is an increasing of electric field intensity near protuberances both in external and self-formed electrical field: the higher is the curvature of surface the stronger is the intensity of near surface electrical field. Consequently two competing processes occur of surface molecules mass transfer: both the self-diffusion smoothing of surface molecule concentration and drawing of molecules in the strong electric field regions. Depending on the initial shape of the protuberance either relaxation or instability occurs. There is a critical wavelength $\lambda = RkT/2U$, which shows that shorter wavelength deviations decrease their amplitudes and longer wavelength deviations grow in amplitude by time. Here R is the characteristic of material, T is temperature, and U is the interaction energy of surface molecules with the electric field. Thus the stronger is the electric field (or the higher is the electrical charge on the surface) the shorter wavelength deviations are increasing their amplitudes. Since there are random variations of any surface from the plane form, being placed in an electric field these surfaces will be unstable depending on the intensity of electric field and properties of material.

P3.2

**KINETIC PROPERTIES OF ADATOMS IN SINE-GORDON
MODEL.** I.V. Baryakhtar, Inst. Low Temp. Phys., Kharkov,
UKRAINE.

The dynamics of adatoms attracts steady attention as an example of dynamical behavior of low dimensional systems. In this paper kinetic properties of 1D adatoms structures are considered. The one dimensional line type of adatoms ordering is of a special interest because it was investigated experimentally well enough, for example, by electron and neutron scattering on such structures in 2D crystals. 1D adatom structures can be formed on the anisotropic substrates. La atoms on the W substrate and atoms of inert gas on the graphite substrate are well known examples of line type ordering. When the amplitude of periodic potential of substrate U is much less than averaging energy of the adatoms interaction J , the Hamiltonian of adatoms displacement can be reduced to well known Sine-Gordon model, which is exactly integrable model. One soliton or kink type solution of Sine-Gordon describes 1D adatom structure, two-soliton solution can be interpreted as bound state of two adatom structures. Common property of solitons in the exactly integrable systems is their interaction without change of the velocity and the only result is the shift of their coordinates. The specific type of solitons interaction in the frame of Sine-Gordon model, as well as in the other exactly integrable models, leads to principally different kinetics as compared with usual particles or quasiparticles. In particular, the main mechanism of relaxation is soliton-soliton collisions with shifts of coordinates. This property takes place in the systems close to the integrable ones also. Here the kinetic equation for a system of 1D adatom structures has been constructed and self-diffusion and internal friction coefficients have been calculated. The process of adatoms homogenization is discussed.

P3.3

**COUPLING OF THERMAL GROOVING AND MIGRATION OF
INCLINED GRAIN BOUNDARIES.** Huifang Zhang, Harris Wong,
Louisiana State Univ, Dept of Mechanical Engineering, Baton Rouge,
LA.

Grain boundary migration is a fundamental process governing grain growth. The motion of a grain boundary is significantly affected by the presence of a free surface because of the formation of a groove at the triple junction. The interaction of grain boundary migration and thermal grooving has not been studied in detail. We have coupled

thermal grooving and grain-boundary migration for slightly inclined grain boundaries, and obtained free-surface and grain-boundary profiles. We assume that thermal grooving results from surface diffusion whereas grain boundary migration obeys a curvature-driven law of motion. A range of length and time scales are needed to describe the coupled motion. It is found that the grain boundary is never pinned. We will present these results and discuss the implications.

P3.4

Abstract Withdrawn.

P3.5

**THE CHEMISORPTION AND DIFFUSION OF OXYGEN AT
DEFECTED Al(111) SURFACES.** Nabanita Majumdar, University of
Virginia, Dept of Material Science and Engineering, Charlottesville,
VA; M. Neurock, University of Virginia, Dept of Chemical
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VA.

The oxidation of aluminum involves a number of atomic steps including molecular dissociation, chemisorption and atomic diffusion. Here the chemisorption and diffusion of oxygen on Aluminum (111) surface is explored with Density Functional Theory calculations. Oxygen molecule dissociates with a large amount of energy (5.0eV) release when the atoms chemisorb into the surface. This energy enables the atoms to overcome the activation barrier for diffusion and play around the surface. The energy barrier for an oxygen atom to diffuse along the surface is computed to be .79 eV. The diffusion into a perfect surface is found to be difficult due to high energy barrier of approximately 2.3 eV. Real aluminum surface contains many growth steps. The DFT method has been used to explain diffusion at a ledge surface. The Oxygen atom trajectory during diffusion to a subsurface position is computed. The activation barrier in this case is found to be 1.2 eV, less than that for a perfect surface case. This appears to be an important mechanism for Oxygen incorporation in an aluminum surface and the formation of the oxide structure.

P3.6

**THE CAPILLARITY INFLUENCE ON SHAPE OF SMALL LIQUID
INCLUSIONS ENCLOSED IN A SOLID UNDER NON-
STATIONARY THERMAL CONDITIONS.** Vladimir Gershanov,
Sergey Garmashov, Andrey Minyaev, Nickita Ivanov, Irina Nosuleva,
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The shape of small liquid inclusions enclosed in an anisotropic solid changes under the action of weak ($< 10^{-3}$) temperature oscillations. This effect takes place due to the anisotropy of interface kinetics, so that it can be used to determine the mechanism of interface processes from the analysis of inclusion shape behavior under various non-stationary thermal conditions. Besides, the possibility of controlling inclusion shape under temperature oscillations is of a great interest for fabrication of 3d p-n-junctions of complicated configuration by thermomigration method. However the small sizes of the inclusions cause a profound influence of capillarity on the inclusion shape controllability under temperature oscillations: the inclusion shape ceases to change as soon as it attains certain limit sizes. In some particular cases, the limit shape of liquid inclusion can be calculated analytically. In general, the considered problem requires the numerical simulation. The evolution of cross-sectional shape of liquid cylindrical inclusion enclosed in uniformly heated crystalline wafer has been numerically simulated in order to determine domains of applicability of analytical model, to calculate the limit shapes and the duration of cross-section shape change (from equilibrium shape to limit one) under various non-stationary thermal conditions, and to draw the conclusions about the most preferable non-stationary thermal conditions for faster and greater change of inclusion shape. It has been shown that the inclusion shape controllability under temperature oscillations has improved with decreasing of the process average temperature.

P3.7

MODELLING LAYER-BY-LAYER GROWTH IN IBAD.
Jussi Sillanpää, Accelerator Laboratory, University of Helsinki,
Helsinki, FINLAND; Ismo Koponen, Department of Physics,
University of Helsinki, Helsinki, FINLAND.

We present a simple rate equation model for layer-by-layer growth in ion beam assisted deposition. Adatom and island diffusion, island detachment and breakup, coalescence of large islands and interlayer transitions of adatoms are taken into account and their effect on growth is studied. We use our computer simulations to gauge the relative importance of different atomic processes in promoting layer-by-layer growth.

P3.8
CALCULATION OF THE DIFFUSION COEFFICIENT OF EQUILIBRIUM SYSTEMS WITH ATTRACTIVE INTERACTIONS. Eleni Arapaki, Panos Argyrakis, Department of Physics, University of Thessaloniki, Thessaloniki, GREECE; Michael C. Tringides, Department of Physics and Astronomy and Ames Laboratory, Iowa State University, Ames, IA.

We study using Monte Carlo simulations the behavior of a lattice gas model with attractive nearest neighbor interactions. After the system is quenched to a final temperature T , it evolves in time from an initial random state to attain the (1x1) ordered state. When equilibrium is reached we calculate the circularly averaged structure factor and the autocorrelation function of the above quantity. We estimate the time constants of the autocorrelation function for various temperatures of the system, ranging from $0.8T_c$ to $0.9T_c$. It is possible to relate the fluctuations around the average value of to the microscopic mechanisms present and use the autocorrelation function for the calculation of the diffusion coefficients of the system.

P3.9
AC DRIVEN MORPHOLOGICAL CHANGES OF A CRYSTAL SURFACE. Michel I. Haftel, Naval Research Laboratory, Washington, DC; and Olivier Pierre-Louis, UJF Grenoble, FRANCE and University of Maryland, College Park, MD.

The "AC" driving of a surface with temperature, a perpendicular electric field, or an elastic strain, share similarities with parametric oscillators and "ratchets". An external AC driving force can lead to mound formation, or flatten the surface. Using a general formulation based on the Burton Cabrera and Frank step model, we describe how the AC driving force leads to morphological changes. On the basis of kinetic Monte Carlo (KMC) simulations, the variation of roughening and lateral coarsening exponents with amplitude and frequency are calculated. As a quantitative example, we consider AC variations in electrochemical potential. Using surface embedded atom method potentials to calculate the dependence of transport constants on metal surfaces on the electrochemical potential, we show that the AC changing of the polarity of the potential with respect to the potential of zero charge can drive the surface toward either stability or instability with respect to mounds, and this is verified in KMC simulations. We present illustrations of the nanopatterned surface from the KMC simulations driven by these AC influences.

P3.10
INFLUENCE OF EPILAYER THICKNESS ON THE STEP-BUNCHING INSTABILITY IN STRAINED SYSTEMS. Alexander C. Schindler, The Blackett Laboratory, Imperial College, London, UNITED KINGDOM; Mark Gyure, HRL Laboratories, Malibu, CA; Dimitri D. Vvedensky, The Blackett Laboratory, Imperial College, London, UNITED KINGDOM.

Strain has proven to play a major role in the evolution of surface morphologies of heteroepitaxial systems. Based on the general approach of continuum elasticity as presented in [1], we have developed a method for the calculation of strain effects in lattice mismatched systems. This method allows us to self consistently calculate quantities like the strain-energy density for any given surface configuration at any given point by specifying only the elastic constants of the involved materials and the boundary conditions. In this model, step velocities are determined from the equilibrium adatom density and the strain-energy at the step edge. This model was applied to the interesting problem of step-bunching during growth on vicinal surfaces, and especially for the case of thin films. Comparing to previous results by Tersoff et al. [2], we find that the step-bunching process due to a logarithmic attraction of steps is observed only in the asymptotic limit of a homogeneously strained substrate, belonging to the limit of a semi-infinite, dislocation free buffer layer between substrate and epilayer surface. In the experimentally relevant case of the growth of relatively thin epilayers, we observe that due to elastic interactions, the morphology of the underlying substrate plays a crucial role for the evolution of the epilayer surface.

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[2] J. Tersoff, Y.H. Phang, Z. Zhang and M.G. Lagally, Phys. Rev. Lett. **75**, 2730 (1995).

P3.11
MODEL FOR DOPANT AND IMPURITY SEGREGATION DURING VAPOR PHASE GROWTH. Craig B. Arnold and Michael J. Aziz, Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA.

We propose a new kinetic model for surface segregation during vapor phase growth that takes into account multiple mechanisms for segregation, including mechanisms for inter-layer exchange as well as

surface diffusion. The resulting behavior of the segregation length shows temperature and velocity dependence, both of which have been observed in experiments. We compare our analytic model to experimental measurements for segregation in silicon based systems and we find a good agreement using realistic energies and pre-exponential factors for kinetic rate constants.

P3.12
ATOMIC MIGRATION AT HIGHLY STRESS REGION BY HYDROGEN ANNEALING. Ju-Wook Lee, Jeongyong Lee, Korea Advanced Institute of Science and Technology, Dept of Materials Science and Engineering, Tae-jon, KOREA.

Atomic migration at highly structural stress region of trench during hydrogen ambient thermal annealing was investigated using high resolution transmission electron microscopy with atomic scale view. Migrated atoms at convex and concave corners formed specific crystal planes such as (111), (113) low index planes, instead of fully rounded corners to reduce the overall surface energy. We could observe the buildup of migrated atoms against the oxide mask, which originated from the surface migration of silicon atoms. Using this hydrogen annealing, more uniform thermal oxide having smooth interface with silicon substrate could be grown on trench surfaces, suitable for the improvement of oxide breakdown.

P3.13
SPIRAL GROWTH IN MOLECULAR BEAM EPITAXY FAR FROM THERMODYNAMIC EQUILIBRIUM: SCALING BEHAVIOR AND GROWTH MODE TRANSITIONS. Karin Wiesauer and Gunther Springholz, Johannes Kepler Universitaet, Linz, AUSTRIA.

The formation of growth spirals on the surface of epitaxial layers is a wide spread phenomenon in lattice-mismatched heteroepitaxy which has been observed for a large variety of different materials systems, ranging from high T_c superconductors to semiconductors including GaAs, InP, GaSb, GaN, and PbTe. Spiral growth is mediated by the existence of screw type dislocations and it is well known for bulk single crystal growth under conditions close to thermodynamic equilibrium. It can be described by the Burton-Cabrera-Frank (BCF) growth theory, predicting the step spacings within the growth spirals in terms of the supersaturation and critical island size of the growth system. In lattice-mismatched hetero-epitaxy of thin films, growth spirals are usually a consequence of the high density of threading dislocations that are formed during the strain relaxation process. In this case, however, deposition is usually carried out far from thermodynamic where the BCF model should not be applicable. Here we have performed a systematic growth study for PbTe molecular beam epitaxy on BaF₂ (111) substrates, which is largely dominated by the high density of growth spirals formed after strain relaxation. We find that the step spacing is more than two orders of magnitude larger than the critical island size and it exhibits a completely different scaling as a function of growth rate than expected from the BCF theory, with a scaling exponent of $\alpha=1/3$ as compared to $\alpha=1$ according to the BCF model. Even more, at very high growth rates a break down of the spiral growth mode is observed with a transition to a 2D layer-by-layer growth mode. This strong deviation is due to the strong coupling of the surface step motion by adatom surface diffusion fields (1). The same effect was even observed for high temperature epitaxial growth, where a significant amount of re-evaporation takes place. This indicates that even under such conditions, surface diffusion is of crucial importance for epitaxial growth.

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P3.14
BOUNDARY CONDITIONS FOR ADATOM DIFFUSION IN EPITAXIAL GROWTH. Russel Caffisch and Cameron Connell, UCLA, Dept. of Mathematics, Los Angeles, CA.

Simulation of epitaxial growth, for example by the island dynamics/level set method [1], requires boundary conditions on step edges (or island boundaries) for diffusion of the adatom density. We start from a model for step edge dynamics [2] that is a generalization of the classical theory of Burton-Cabrera-Frank to nonequilibrium growth, as required for MBE applications. This theory includes dynamics of edge adatoms and kinks on the step edge, in addition to adatoms on the terraces. From this model, we derive a curvature term in the boundary condition, as in the Gibbs-Thomson law, as well as a second derivative of curvature term in the formula for velocity of the boundary. Computational results with this boundary condition are compared with results from using the full step edge dynamics model, as well as with results from an irreversible aggregation model and from kinetic Monte Carlo simulations.

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P3.15

EVOLUTION OF SURFACE STRESS DURING GROWTH OF COBALT SILICIDE ISLANDS BY REACTIVE DEPOSITION. D.G. Waters, G.J. Nivison, T.H. McDaniels and P.A. Bennett, Dept. of Physics and Astronomy and Science and Engineering of Materials, Arizona State University, Tempe, AZ.

We report in situ measurements of surface stress during formation of silicide islands by reactive deposition. Island structures (coverage, aspect ratio, and coalescence) are determined ex situ using TEM and AFM. For growth on Si(111) at $T > 600\text{C}$ we observe a surface stress $\sigma = 0.5\text{N/m}$ per MI (tensile) in the observed range of 0-10MI in close agreement with calculations for a fully coherent film of CoSi/sub2. For $T = 500\text{C}$, we observe $\sigma = -0.2\text{N/m}$ per MI (compressive), which is attributed to partially coherent CoSi(CsCl), a metastable phase with lattice mismatch of 0.9%. For $T = 200\text{C}$ σ alternates through several cycles of compressive/tensile stress in the coverage range 0-20 MI. This is attributed to a sequence of silicide phases vs coverage. On Si(100), we observe $\sigma = 0.15\text{N/m}$ per MI for all T in the range 25 - 800C. This low value of stress is attributed to a mixed orientation of CoSi/sub2, which surprisingly is independent of growth temperature.

P3.16

DEVELOPMENT OF EXTREMELY HIGH LEVELS OF STRESS DURING DEPOSITION OF FULLERENE-LIKE CN_x THIN FILMS BY UN-BALANCED MAGNETRON SPUTTERING WITH LOW ION ENERGY BOMBARDMENT. Ian Brunell, Jörg Neidhardt, Zsolt Czizgány, Lars Hultman, Thin Film Physics Division, Department of Physics (IFM), Linköping University, Linköping, SWEDEN.

It is well known that high stress levels play an important role in adhesion and mechanical failure of thin films. However, there have been few reports on the stresses in the recently discovered fullerene-like CN_x thin films and the effects of deposition parameters. We have investigated the effects of deposition parameters upon stress development of CN_x thin films in-situ during growth. Thin films ≈ 500 nm thick were deposited by un-balanced, reactive, magnetron sputtering in an Ar/ N_2 atmosphere. The radius of curvature was monitored by laser deflection technique during deposition which is related to the stress in the deposited film. The effects of substrate temperature, ion energy, and ion to atom arrival rate ratio were investigated. The micro-structure was investigated by TEM, the composition by AES, and the mechanical response to nanoindentation was recorded. It was found that the stress is initially tensile then, after ≈ 200 s (20 nm), it becomes compressive, reaching a maximum of as much as 7 GPa, and then relaxing slightly. The maximum stress during growth varies with substrate temperature; the peak value is observed at 300°C. It is remarkable that such high levels of stress were observed for such low ion energies, ≈ 28 eV, and such low ion-to-neutral arrival rate ratio (typically < 1). In comparison, deposition of pure carbon films under similar conditions yielded much lower stress levels, typically 1 GPa. We believe this effect is related to the textured fullerene-like microstructure of the CN_x films, which consist of curved, standing, basal-planes. The compressive stress build-up is postulated to be due to the Gibbs-Thomson effect as the basal planes close upon themselves in the plane of the film.

P3.17

MOLECULAR-DYNAMICS STUDIES OF VOID GROWTH IN STRAINED DUCTILE METALLIC THIN FILMS. M. Rauf Gungor and Dimitrios Maroudas, Dept. of Chemical Engineering, Univ. of California, Santa Barbara, CA.

The dynamics of failure in strained ductile metallic thin films is governed by various stress relaxation mechanisms mediated by formation and propagation of crystalline defects including point defects, dislocations, and larger-scale defects such as voids. In this presentation, stress relaxation due to void growth is analyzed based on atomic-scale simulation. The analysis focuses on copper thin films under conditions of tensile thermomechanical strain that are representative of those experienced by metallic thin films used in device interconnections in integrated circuits. In our atomistic simulations, the interatomic interactions are described by an embedded-atom-method (EAM) parametrization for copper. Molecular-dynamics (MD) simulations are carried out using large, million-atom supercells with cylindrical voids that extend throughout the thickness of the thin film. Results of MD simulations are presented over a range of residual thermal tensile strains and thin-film temperatures for given crystallographic orientation of the film surface. Relaxation of the tensile stress in these ductile copper films is found to occur through void growth mediated by plastic deformation and self-diffusion mechanisms. Dislocation emission from the surface of the void and subsequent dislocation propagation through the film are demonstrated and their role in void growth and stress relaxation is analyzed in detail. In addition, mechanisms of nanovoid nucleation and growth ahead of larger voids are analyzed that can lead to film

rupture at high tensile strains. The MD simulations suggest a possible delamination mechanism that can be initiated in devices at interfaces between the metal and soft dielectric materials due to interface roughening induced by plastic deformation in the film. The atomic-scale simulation results are used to parametrize phenomenological kinetic models of strain relaxation: the model parameters depend on the stress level and the mode of deformation. The results of our kinetic analysis are incorporated into continuum-scale self-consistent dynamical models of electromechanically-induced thin-film failure. Implications of the multi-scale modeling results for copper interconnect reliability also are discussed.

P3.18

MICROSTRUCTURE EVOLUTION IN THIN FILM AND NEAR SURFACES: PHASE FIELD MICROELASTICITY APPROACH. Yongmei M. Jin, Armen G. Khachaturyan, Rutgers Univ, Dept of Ceramics and Materials Engineering, Piscataway, NJ.

The elastic strain generated by the coherent phase transformation is significantly modified by the image force effect near free surfaces and in thin films. This effect is explicitly taken into account by extension of the Phase Field Microelasticity (PFM) approach, which is based on the exact solution of the elasticity equation for an arbitrary structurally inhomogeneous system of elastically homogeneous half-infinite macroscopic uniform body. Being incorporated in the Phase Field formalism, this solution provides the computational model that is as efficient as the existing PFM model for the bulk systems. This modified theory makes it possible to realistically simulate the 3-D evolution of the coherent multidomain and multiphase microstructures as well as mobile defects in a vicinity of free surface and in deposited thin films. The Phase Field model of phase transformation near free surface, as any Phase Field model, does not impose *a priori* geometrical and structural constraints on possible microstructure evolution path. The model is used to investigate the specific features of microstructure evolution and its interactions with defects associated with free surfaces. The image-force-induced heterogeneous nucleation and the influences of various defects, such as precipitates and dislocations, on the development of mesoscopic morphology of phase transformation in thin film are simulated. Examples of 3D simulation are discussed.

P3.19

IN SITU STUDY OF TITANIUM FILM GROWTH ON DIFFERENT SUBSTRATE SURFACES. Paul Oberhauser and Reinhard Abermann, Univ of Innsbruck, Inst of Physical Chemistry, AUSTRIA.

The growth of thin Ti-films on different substrate surfaces was investigated under UHV-conditions by in situ internal stress measurements. The main objective of these experiments was to investigate the influence of the chemical and microstructural properties of the substrate on thin film growth. The first substrate used was a highly crystalline TiO_2 -film prepared by reactive evaporation of Ti in an oxygen atmosphere and subsequent annealing*. The Ti-growth stress on this substrate is compressive up to monolayer coverage and tensile at higher film thickness, which is interpreted to indicate a strong interaction between TiO_2 and the arriving Ti atoms at the interface during monolayer formation and strained (tensile) layer epitaxy at higher film thickness. In a second series of experiments the TiO_2 -film was covered with Al-overlayers of increasing thickness. Due to oxygen interdiffusion from the TiO_2 -film an amorphous Al-oxide layer is formed at the interface eliminating the high degree of order in this film. On this substrate the stress curve of the Ti-film shows increasing tensile stress at low and compressive stress at high thickness. Thus a few monolayers of Al give rise to a transition from epitaxial to polycrystalline Ti-film growth. Increasing the thickness of the Al-overlayer eventually produces a metallic Al-surface. The structure of this surface depends on the film thickness and substrate temperature during its deposition. The stress vs. thickness curve of the clean Ti-film growing on this surface shows two features: (i) A tensile stress during deposition of the first Ti-monolayer (with an incremental stress up to 44 GPa). Its magnitude is strongly influenced by the morphology of the Al-surface and the Ti-deposition temperature. The structure deduced from the changes in this tensile stress will be compared with that seen on AFM-micrographs. (ii) A tensile stress contribution (with an incremental stress up to 4 GPa) is attributed to alloy formation. Onset and magnitude of this latter tensile stress depend on the Al-film thickness and substrate temperature during Ti-deposition. Planview TEM-micrographs and TED-results will be shown. For comparison, analogous experiments were made with $\text{Al}_2\text{O}_3/\text{Al}$ substrate bilayers. The results of these experiments qualitatively agree with those on the TiO_2/Al -substrate. The general shape of the stress vs. thickness curve is comparable, however quantitative differences are interpreted to show that oxygen interdiffusion from the substrate into the growing Al-film is negligible.

* P. Oberhauser, R. Abermann, Thin Solid Films 350 (1999) 59

P3.20

IN SITU INVESTIGATION OF $TiAl_x$ FILM GROWTH AS A FUNCTION OF SUBSTRATE TEMPERATURE AND FILM STOICHIOMETRY. Stefan Lackner and Reinhard Abermann, Institute of Physical Chemistry, University of Innsbruck, AUSTRIA.

The growth of $TiAl_x$ -alloy films was investigated by measuring the film stress during as well as after the film deposition under UHV-conditions with a cantilever beam technique. The alloy films were deposited from two separate evaporation sources. To cover possible contamination layers on the bending beam an alumina film - prepared by reactive evaporation of Al in an oxygen atmosphere - was used. The substrate temperature (T_s) was varied from room temperature to 500°C and the alloy stoichiometry from $TiAl_3$ to Ti_3Al . At $T_s=500^\circ C$ the film stress is compressive and the dependence on stoichiometry is rather small. Only the stress vs. thickness curve of $TiAl_3$ films shows unexpected oscillations during growth while at lower aluminium content stable stress curves are measured. The stress changes after deposition are large in each case, interpreted to indicate film recrystallisation. While the Ti_3Al -phase was identified by TED results a positive identification of the $TiAl_3$ -phase was not possible. In a further series of experiments the growth stress of Ti_3Al films was investigated at $100^\circ C < T_s < 400^\circ C$ and shows a transition from tensile to compressive stress with small stress changes after deposition. This transition is also reflected in the TEM microstructure of these films. The effect of changes in alloy-stoichiometry was investigated at $T_s=200^\circ C$. At low film thickness the stress vs. thickness curves are similar, however, at film thicknesses above 40nm they differ significantly and show either tensile ($< 20N/m$) or compressive ($> -20N/m$) stresses in 150nm thick films depending on film stoichiometry. These differences in the growth stress are again reflected in the TEM microstructure of the respective films. The effect of heating these low-temperature-films to 500°C will be discussed.

P3.21

ON THE EFFECT OF STRAIN ON THE ACTIVATION ENERGY FOR ADATOM MIGRATION. Alonso D. Peralta, Mechanical Engineering Department, State University of New York, Stony Brook, NY.

The effect of strain on the activation energy for adatom migration is considered. Mechanical strain may develop in thin films as a result of lattice mismatch, surface and internal defects, and from externally applied strains, amongst others. Such strain affects the chemical potential of the surface. In the case of a uniformly distributed strain (or stress), it is well known that such strain fields can lead to surface instabilities. These instabilities can be explained in terms of energy considerations of the system. Furthermore, depending on the sign of the uniform strain, diffusion may be either enhanced or decreased. This effect is believed to be the result of a change in the diffusion coefficient as a result of the applied strain. It is shown here how uniform and non-uniform strains affect the activation barrier for adatom migration. The change in diffusion coefficient may then be related to the change in the activation barrier.

P3.22

ATOMISTIC MODELS FOR THE SURFACE STRESS OF FCC METALS WITH APPLICATION TO SURFACE RECONSTRUCTIONS. T.M. Trimble and R.C. Cammarata, Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, MD.

The surface stress is a thermodynamic quantity associated with the reversible work per unit area to elastically stretch a free solid surface. This is in contrast to the related quantity surface free energy, which is equal to the reversible work per unit area to create a new surface by, e.g., fracture. We have investigated the link between these two quantities and the macroscopic quantities cohesive strength, the bulk modulus B , and the shear modulus G using pair-potentials and an embedded atom potential (EAM). The surface properties were investigated analytically for unrelaxed surfaces, and by computer simulation for fully relaxed surfaces. Pair-potentials are inherently unable to describe real metal surface because they neglect many-body effects. However, it is possible to use an analytic form of the EAM potential to obtain behavior in good qualitative and quantitative agreement with first principle calculations. It will be shown that for (111) and (100) oriented surfaces of several fcc metals, there is a correlation between the relative magnitudes of the surface stress and surface free energy and the ratio B/G . This correlation is then used to discuss the stability of clean metal surfaces to surface reconstructions. It will be shown that many features of the reconstruction behavior can be well reproduced by computer simulations using the analytic EAM potential, and is also in good agreement with a simple continuum thermodynamic model involving the surface stress, surface free energy, shear modulus, and lattice parameter.

P3.23

DETERMINATION OF g-FACTOR VALUES OF ULTRATHIN FILM $Fe/InAs(100)$ BY BRILLOUIN LIGHT SCATTERING. Guang-Xu Gheng and Hong-Ru Zhai, Laboratory of Solid State Microstructures and Center of Materials Analysis, Nanjing University, Nanjing, CHINA; Ya Zhai, Dept of Physics, South East University, Nanjing, Jiangsu, CHINA; Y.B. Xu, E.T.M. Kernoham and J.A.C. Bland, Cavendish Laboratory, University of Cambridge, Cambridge, UNITED KINGDOM; Jia Cheng, Department of Electronic Engineering, Shanghai Jiaotong University, Shanghai, CHINA.

The magnetic properties of ultrathin films of various thickness deposited on $InAs(100)$ substrate in UHV with a multi-technique molecular beam epitaxy (MBE) system have been studied by Brillouin Light scattering (BLS). The evolution of in-plane magnetic anisotropy with changing thickness of the Fe film is seen, consistent with the result of in-situ magneto-optical Kerr (MOKE) loop observation¹. A dominant and in-plane producible fourfold magnetic anisotropy was clearly present in $Fe(100ML)/InAs$ from the magnon (spin wave) frequency ω (GHz) versus orientation angle Θ (degree) of the in-plane applied magnetic field. When the thickness of Fe layer is decreased the reduction of the in-plane magnetic anisotropy appeared. For $Fe(8ML)/InAs$ the fourfold anisotropy is obviously broken down. It is interesting that the g-factor value of Fe film is reduced to about 7/10 of the value in $Fe(100ML)$. Some possible interpretations is given.

Reference:

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P3.24

MAGNETIC AND RESISTANCE MEASUREMENTS ON BORON-DOPED AND UNDOPED Ni_3Al THIN FILMS. Edward Patterson, Laurence L. Henry, Southern University and A&M College, Baton Rouge, LA.

We report preliminary results of magnetization and I-V measurements of the effects of boron doping on the magnetic and electron transport properties of Ni_3Al thin films. Magnetization and resistance measurements in magnetic fields up to 5 T were performed on 500 Å (nominal) thick films that were fabricated by ion beam sputtering of compound targets. Both a doped (~200 ppm B) and undoped film were investigated. For the boron-doped film, the magnetization is enhanced with a broad transition that occurs in several stages over the temperature range from 27 K to 56 K. Further, as the temperature is increased through the transition range dM/dT fluctuates between negative and positive values, and the magnetization changes from positive to negative near $T = 52$ K. Results of four probe I-V measurements performed on the samples with the current in the plane of the film, and an applied magnetic field parallel to the plane of the film, are consistent with these results. In addition, magnetoresistance (magnetic field = 50 G and 5T) measurements with the current applied "perpendicular" to the magnetic field show a transition from non-metallic to metallic behavior for the undoped sample in the 190 K - 230 K temperature range. This transition is not seen in the doped sample.

Work supported by grants from the LEQSF, the Dept. of Physics at Southern University and A&M College, Baton Rouge campus, and NASA.

P3.25

CRYSTAL STRUCTURES OF Mn AND Fe THIN FILMS GROWN ON GaAs (001) SUBSTRATES DETERMINED BY SYNCHROTRON RADIATION X-RAY DIFFRACTION. Y.Z. Wu, D. Qian, W.X. Tang, D. Wu, G.S. Dong and X.F. Jin, Surface Physics Laboratory, Fudan University, Shanghai, CHINA; Q.J. Jia and X.M. Jiang, Synchrotron Radiation Laboratory, Institute of High Energy Physics, Chinese Academy of Science, Beijing, CHINA.

The correlation between the crystal structures and the magnetic properties of the magnetic materials is believed to be important in understanding the origin of the magnetism. The development of molecular beam epitaxy technique allows epitaxial growth of various stable and metastable phases of 3d metals and alloys on semiconductor substrates, which provides a way to prepare the samples for such correlation studies. Here we report the studies of the crystal structures of the Mn and Fe thin films grown on GaAs (001) substrates measured by synchrotron radiation X-ray diffraction. The results indicate that the Mn thin films grown at 400K have a face-centered-cubic-like structure. The in-plane lattice constant of such Mn film determined by grazing angle incident X-ray diffraction is $a=0.3821nm$, and the out-plane lattice constant determined by large angle incident X-ray diffraction is $c=0.3728nm$. The ratio of a to c is about 1.02. This indicates that the crystal structure of Mn on GaAs (001) is very close to a fcc structure, one of the metastable phases of bulk metal Mn. For the case of Fe on GaAs (001) substrates, the lattice constants are $a=0.2829nm$ (in-plane) and $c=0.2909nm$ (out-plane) respectively. The ratio of a to c is about 0.97. Clearly the structure of Fe thin film on GaAs (001) is close to a bcc structure.

Besides, the standing wave configurations also were clearly observed in the X-ray diffraction intensity profiles from Fe thin films, which implies that the Fe thin films have a high-quality with atomically smooth level. The atomic layer spacing in the direction perpendicular to the surface of Fe thin films deduced from the nodal position of the X-ray standing wave is 0.1457nm, which is consistent with the data of lattice constant deduced from the position of the X-ray diffraction peak.

P3.26

ENHANCED ELECTRICALLY-INDUCED NONVOLATILE RESISTANCE CHANGE IN MAGNETORESISTIVE FILMS BY POST-ANNEALING. Shangqing Liu, Najuan Wu, Alex Ignatiev, Space Vacuum Epitaxy Center and Texas Center for Superconductivity, University of Houston, Houston, TX.

Colossal Magnetoresistive (CMR) thin films have shown a large electric-pulse-induced resistivity (EPIR) change effect in zero magnetic field and at room temperature. The resistance of such films can be both decreased and increased through multiple nonvolatile intermediate levels by short electrical pulses. An enhancement of this effect has been seen for $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_7$ (PCMO) films grown by pulsed laser deposition as the result of film annealing. PCMO films that had been previously studied and hence switched in resistance by pulsing were subsequently annealed at 170°C in air for 0.5 hr. Upon cooling the films showed increase in the nonvolatile resistance ratio $\Delta R/R_{\text{min}} = (R_{\text{max}} - R_{\text{min}})/R_{\text{min}}$ by more than 700%.

P3.27

MAGNETICS THIN FILMS PREPARED BY SOL-GEL PROCESS. Luciana Seara, Nelcy Della Santina Mohallem, Federal University of Minas Gerais, Dept of Chemistry, Belo Horizonte, BRAZIL.

Nanostructured particles have been researched due to their high surface/volume ration, which gives them unique properties diverse from those of similar polycrystalline materials. The use of an inorganic matrix as a host for this nanocrystalline particles has been demonstrated to be a form of getting uniform size distribution. Silica has been used as a matrix material due to its high thermal and chemical stability. Magnetic composites formed by metallic oxide dispersed in a ceramic matrix has been studied to produce catalysts, sensors, and optical-magnetic devices. In this work, nickel ferrite thin films and magnetic composite thin films formed by nickel ferrites disperse in a silica matrix were prepared by sol-gel process using metallic nitrates as a precursor of the ferrite and tetraethylorthosilicate (TEOS) as a precursor of silica. The composite films were obtained with different contents of ferrite. All the films were prepared and deposited on glass plates using the dip-coating process and they were adherent, transparent, homogeneous and free of microcracks. Film thickness and processes parameters such as ferrite concentration, dipping velocity, solution viscosity and heat treatment temperature were correlated and associate with the coating morphology and magnetic properties. The composition of the films was determined by X-ray fluorescence using synchrotron radiation. The morphology was studied by atomic force microscopy and the magnetic behavior by magnetic force microscopy. Porosity and refraction index were estimated by spectroscopy UV/visible.

P3.28

PERPENDICULAR MAGNETIC ANISOTROPY IN ULTRATHIN YIG FILMS PREPARED BY PULSED LASER DEPOSITION TECHNIQUE. Elena Popova, Niels Keller, Marcel Guyot, Marie-Claire Brianso, Michel Tessier, Versailles University, LMOV, Versailles, FRANCE; Francois Gendron, Pierre and Marie Curie University, LMDH, Paris, FRANCE.

The development of high frequency and magneto-optical memory devices increases the interest in thin ferrite film preparation and investigation of their physical properties. A change of these properties is expected when the film thickness becomes of the order of a few lattice parameters. We report on thin and ultrathin yttrium iron garnet (YIG) film preparation by pulsed laser deposition technique. The films deposited on the quartz substrates are polycrystalline with slightly distorted lattice, though the average lattice parameter is the same as for bulk YIG (12.376 Å). The bulk Curie temperature of 557 K is observed for these films by means of magneto-optical Faraday rotation measurements. However, the saturation magnetization is slightly inferior to the bulk value in the range of 5 - 380 K. Ferromagnetic resonance (FMR) studies of samples with thickness 100 - 3800 Å were performed in different measurement geometries and in the temperature range of 3.5 - 300 K. We observed a change of sign of the effective magnetization ($4\pi M_e f f$) appearing below a film thickness of approximately 120 Å. The inversion of the easy magnetization direction from in-plane to out-of-plane, i.e. the perpendicular magnetic anisotropy becomes evident above a cross-over temperature which is thickness-dependent. The effective magnetization for a given temperature decreased with decreasing

sample thickness. This can be caused by an increasing contribution of the surface anisotropy to $4\pi M_e f f$ when the sample thickness is reduced.

P3.29

EPITAXIAL GROWTH OF (001) AND (111) Ni FILMS ON MgO SUBSTRATES. R.A. Lukaszew, V.A. Stoica, C. Uher and R. Clarke, Physics Department, University of Michigan, Ann Arbor, MI.

Metal-ceramic interfaces are important in applications as diverse as magnetic storage media [1] or supported catalysts. [2] It is very important to understand how the crystallography and microstructure of the films depend on growth and/or annealing conditions so that other physical properties (e.g. magnetic, electronic, etc.) can be tailored for specific applications. We will present our studies on the epitaxial growth and annealing of (001) and (111) Ni films MBE grown on MgO substrates. We have observed the evolution of the surface using correlated in-situ RHEED (reflection high-energy-electron diffraction) and STM (scanning tunneling microscopy) measurements. In particular we found that annealing a 30.0 nm (001) Ni film at 250°C improves the roughness from 2.0 nm to 1.0 nm. We have noticed that RHEED shows 2x1 reconstruction for the (001) films, but no reconstruction is observed for (111) films. We will also show our preliminary magnetic anisotropy studies on these films using MOKE. [1]. J.K. Howard, J. Vac. Sci. Technol. A 4 (1986) 1. [2]. J.E.E. Baglin, G.J. Clark, J.F. Ziegler, Nucl. Instrum. Meth. 218 (1983) 445.

P3.30

DEPOSITION-ORDER-DEPENDENT MAGNETIC PROPERTIES OF CoNi/Gd BILAYERS. B. Altunçevahir and A.R. Koymen, Department of Physics, University of Texas at Arlington, Arlington, TX.

CoNi films were grown on thin Gd underlayers at room temperature using DC magnetron sputtering. A large change in the coercivity of CoNi/Gd bilayer system was observed and this increase in coercivity was not seen when film growth order was reversed for the same thicknesses. The increase in coercivity strongly depends on the composition ratio of the Co and Ni. Based on the initial magnetization and angle dependent coercivity measurements, the increase in the coercivity is attributed to the domain pinning sites developed in the interface of the CoNi and Gd. The cause and mechanism of these pinning sites are currently under investigation. However it is expected that these sites develop due to the decrease of the Ni moment as a result of charge transfer from Gd.

P3.31

STRAIN DEPENDENCE AND MAGNETIC ANISOTROPY IN CHROMIUM DIOXIDE THIN FILMS. L. Spinu, H. Srikanth, University of New Orleans, Advanced Materials Research Institute, New Orleans, LA; A. Gupta, IBM T.J. Watson Research Center, Yorktown Heights, NY; X.W. Li, G. Xiao, Brown University, Providence, RI.

Field-dependent transverse susceptibility measurements based on a novel tunnel-diode oscillator (TDO) method were used to probe the magnetic anisotropy and switching in CrO_2 films. The thin films grown epitaxially on (100) TiO_2 substrates exhibited a strong in-plane uniaxial anisotropy with the magnetic easy and hard axes lying in the [001] and [010] directions, respectively. Singular peaks in the transverse susceptibility were observed that are associated with the anisotropy and switching fields in CrO_2 . Theoretical calculations based on a coherent rotation model display remarkable agreement with the experimental data indicating that these thin films behave like single domain magnetic particles. The transverse susceptibility data at low temperatures reveal an unusual variation of the singular peaks. This can be described by including magnetoelastic contributions resulting from the in-plane tensile strain in the films due to lattice mismatch with the substrate. We will also discuss the evolution of the anisotropy and switching fields for the full angular dependence of transverse susceptibility. Work at AMRI is supported by the US Department of Defense through DARPA grant No. MDA 972-97-1-003

P3.32

STRESS DEVELOPMENT IN Co/Cu MULTILAYERS. Brennan L. Peterson, Bruce M. Clemens, Robert L. White, Stanford University, Department of Materials Science and Engineering, Stanford, CA.

Giant magnetoresistance observed in cobalt-copper multilayer films has motivated intensive study of their structure and growth. A key consideration in processing, and ultimately understanding these layers is the stress which develops in the film during growth. The stress in the film depends on the surface energy, lattice mismatch, and growth morphology, and thus *in-situ* stress measurement can be a useful tool in understanding the development of film microstructure and surface energy in a growing film. Further, stresses can have a large effect on

the magnetic properties through inverse magnetostriction. DC magnetron sputtered [Co/Cu] multilayer films were prepared in a sputtering chamber with *in-situ* stress measurement capabilities. The first few monolayers of Co show a tensile stress transient of 4-5 GPa, roughly consistent with expected coherency stresses associated with the lattice mismatch. For greater Co thicknesses, the stress decreases but remains tensile. Copper layers show an initial compressive transient of ~ -2.5 GPa, lower than that expected from coherency stresses. Continued Cu growth results in a reduced compressive stress. For a (Co 3 Å)/(Cu 21 Å) film, with 20 bilayers, the total film stress was approximately 1 GPa tensile, which may have implications for device manufacture. Additionally, films grown with In surfactant layers show different stress behavior, implying that the surfactant layer changes the surface energy and/or film microstructure. The roughness and intermixing of films grown with and without In surfactant were characterized by *ex-situ* synchrotron x-ray scattering. These studies of stress and structure with and without surfactant layers have led to a more complete understanding of growth processes and control.

P3.33
STRUCTURAL AND MECHANICAL PROPERTIES OF AMORPHOUS Zr-BASED ALLOY THIN FILMS. S.G. Mayr, I. Physikalisches Institut, Universität Göttingen, Göttingen, GERMANY; M. Moske, Forschungszentrum Caesar, Bonn, GERMANY; K. Samwer, I. Physikalisches Institut, Universität Göttingen, Göttingen, GERMANY.

The evolution of surface structures of coevaporated and sputtered amorphous $Zr_{65}Al_{7.5}Cu_{27.5}$ films with varying deposition conditions is investigated primarily with STM. While vapor deposited thin films reveal pronounced structure formation, depending on parameters, such as substrate temperature, film composition (variation of the Al versus the Cu content) and the angle of incidence, comparable sputtered films hardly show any structure formation. With the help of a numerical analysis of the STM data, surface diffusion, self-shadowing and energy transfer in the case of sputtering can be identified as the main structure forming mechanisms [1]. Presuming these atomic processes, it is possible to model main experimentally observed features of amorphous thin film growth by the use of stochastic continuum growth equations, which are numerically solved [1,2]. Additionally, the connection to intrinsic stress formation during film growth is discussed.

[1] S.G. Mayr, M. Moske and K. Samwer, *Phys. Rev. B* **60** (1999) 16950

[2] M. Raible, S.G. Mayr, S.J. Linz, M. Moske, P. Hänggi and K. Samwer, *Europhys. Lett.* **50** (2000) 61

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P3.34
ELECTROMIGRATION-INDUCED SURFACE WAVE PROPAGATION ON VOIDS IN METALLIC THIN FILMS. M. Rauf Gungor and Dimitrios Maroudas, Dept. of Chemical Engineering, University of California, Santa Barbara, CA.

Failure of metallic thin-film interconnects is among the most important materials reliability problems of solid-state devices used in microelectronics. The dynamics of various failure mechanisms is driven by the mass transport phenomenon of electromigration, which is responsible for the morphological evolution of microstructural defects in these films. The most catastrophic of these defects are transgranular voids, which may propagate across the film under the action of an applied electric field and cause failure. A theoretical non-linear analysis is presented of current-induced morphological evolution of void surfaces in metallic thin films based on self-consistent numerical simulations. Our surface transport model includes capillarity and surface electromigration as driving forces for mass transport and takes into account the surface mobility anisotropy. Surface propagation is computed in a coupled manner with the electrostatic problem in the metallic conductor, which is solved based on a symmetric Galerkin boundary-integral formulation. A systematic parametric study is conducted focusing on cases of low symmetry of surface diffusional anisotropy. The void morphological stability is examined as a function of void size and applied electric field. Our simulations predict a surface morphological transition at a critical electric field strength, which is associated with a Hopf bifurcation. For electric fields weaker than critical, voids of given size migrate along the film at constant speed with steady surface morphologies. For electric fields stronger than critical, voids also migrate along the film at constant speed with surface morphologies that are time periodic. Both of these types of void surfaces are stable and do not lead to film failure. In addition, our simulations have revealed period-doubling bifurcations occurring at higher strengths of electric field for given void size. A comprehensive void morphological stability map is constructed and the onset of failure following surface wave propagation is derived.

P3.35
THE EFFECT OF Pb ON THE INTERFACE STRUCTURE OF Fe/Cr(100) METALLIC MULTILAYERS. Masao Kamiko, Kyu-Young Kim, Sang-Mun Oh, Ryoichi Yamamoto, Institute of Industrial Science, University of Tokyo, Tokyo, JAPAN.

The origin of giant magnetoresistance (GMR) in metallic multilayers is ascribed to spin-dependent scattering caused by the existence of interfaces. Numerous observations have been reported, indicating that interface roughness plays an important role in the GMR effect. However, no clear picture has yet emerged and the reported data are contradictory. Recently, surfactant epitaxy was introduced as a method of changing the growth mode from 3D island growth to the layer-by-layer growth, and successful results were reported. Surfactant epitaxy is a useful method to fabricate flat and abrupt interfaces in metallic multilayer films. To obtain informations about the correlation between structure and electrical property in metallic multilayers, we have fabricated Fe/Cr(100) multilayers with and without Pb as a surfactant by molecular beam epitaxy. We investigated the differences in the interface structures and magnetotransport properties between surfactant-mediated multilayers and normal ones. From the observations of RHEED and High-Resolution X-ray diffraction patterns, we confirmed that the surfaces of Fe/Cr(100) multilayers with Pb are flatter and the interfaces are sharper than one without Pb, which means that Pb operates as an effective surfactant. We have investigated the electrical properties of multilayers by measuring magnetoresistance. The MR ratio of the multilayers prepared with Pb was larger than that of the multilayers prepared without Pb. The change of resistance with magnetic field was larger for the multilayers with a surfactant. This suggests that Pb also changes the magnetotransport property of Fe/Cr(100) multilayers.

P3.36
ELECTRONIC STRUCTURE OF Ag/Cu/Ag/Cu(111) DOUBLE NANOFILM STRUCTURES STUDIED BY ANGLE-RESOLVED PHOTOEMISSION SPECTROSCOPY. Akinori Tanaka, Univ of Rochester, Dept of Physics and Astronomy, Rochester, NY; Kazutoshi Takahashi, Inst of Molecular Science, UVSOR Facility, Okazaki, JAPAN; Hiroyuki Sasaki, Shoji Suzuki, Shigeru Sato, Tohoku Univ, Dept of Physics, Sendai, JAPAN.

Angle-resolved photoemission study of double Ag nanofilm structures, Ag nanofilm (outer nanofilm) / Cu barrier layer / Ag nanofilm (inner nanofilm) / Cu(111) substrate, has been carried out in order to investigate in detail their quantized electronic structures and electronic coupling between the quantized electronic states. An important point to note is that Ag and Cu are lattice-mismatched in the present systems. It is found that the binding energies of the quantized states in the present double Ag nanofilm structures exhibit an avoided-crossing behavior. These experimental results give a direct evidence of coherent electronic coupling between the quantized states in the two Ag nanofilms through a thin Cu barrier layer. This electronic coupling between the quantized states resembles the situation of atomic states, leading to symmetric and antisymmetric combinations of the individual states. Therefore, the energy splitting of the avoided-crossing directly corresponds to twice magnitude of coupling matrix element between the inner and outer quantized states. We have investigated this electronic coupling between the quantized states in the double nanofilm structure with varying Cu barrier layer thickness and inner Ag nanofilm thickness. It is found that the coupling strength between the quantized states, i.e. one half of the energy splitting of the avoided-crossing, increases with decreasing Cu barrier thickness. It is also found that the coupling strength between the quantized states increases with decreasing energy of avoided-crossing relative to Cu sp projected-band edge (increasing binding energy of avoided-crossing with decreasing inner Ag nanofilm thickness). These experimental results are well characterized with a theoretical calculation based on the nearly-free-electron approximation. From these results, we discuss the electronic coupling between the quantized states in the present double Ag nanofilm structures with various configurations.

P3.37
PULSED LASER DEPOSITED NANO CRYSTALLINE ZnO THIN FILMS. Raj K. Thareja, Kumamoto, Kumamoto University, Department of Electrical and Computer Engineering, Kumamoto, JAPAN; Anirban Mitra, Indian Institute of Technology Kanpur, INDIA.

In recent years, there has been a great interest in wide-gap materials because of their potential to produce efficient blue light emitting diodes and short wave length lasers. GaN and its alloys have been a focal point of research in semiconductor and opto electronics industry. One of the problems that has plagued the development of GaN has been the lack of high quality, closely lattice matched materials. Recent works on ZnO has shown it a promising material for UV and blue light emitting devices. ZnO has several other unique properties similar

to indium oxide and tin oxide, it is both transparent in the visible and electrically conductive with appropriate dopant like aluminum or gallium. In the present work, we report on the pulsed laser deposition of ZnO at room temperature (RT). The deposition was done on silicon and glass substrate at RT under the oxygen pressure ranging from 10 mTorr to 1 Torr. We used a frequency tripled third harmonic (355 nm, pulse repetition rate of 10 Hz) of a Nd:Yag laser. The deposited films were characterized using XRD, AFM and PL. The films grown at pressures less than 300 mTorr are found to be highly oriented along (002) plane. The grain size calculated using Scherrer's formula decreases as the pressure of the oxygen gas decreases. Morphology of various films deposited at different background pressure, using AFM, shows that roughness varies from 20 nm to 108 nm. The films grown at lower oxygen pressure are significantly smoother than those grown at higher pressure. The intensity of PL at 395 nm (3.13 eV) is found to depend on the stoichiometry and hence the oxygen pressure. The deposited films were investigated for possible laser action in UV. The sample was optically pumped with 355nm radiation. The pump beam was focused on to the film surface and the lasing was observed through an optical fiber coupled monochromator. A steep rise in the intensity of the emitted spectrum above a certain critical excitation intensity confirmed the laser action. At excitation intensity above threshold, very narrow peaks are observed in the emission spectrum. A detailed investigation of the film and the laser action will be presented.

P3.38

IN-SITU CONDUCTIVITY MEASUREMENTS DURING ANNEALING OF NANOCRYSTALLINE GOLD FILMS MADE BY ADVANCED GAS DEPOSITION. J. Ederth, L.B. Kish, E. Coronel, E. Olsson, and C.G. Granqvist, Department of Materials Science, The Angstrom Laboratory, Uppsala University, Uppsala, SWEDEN.

Recently, nanocrystalline gas-deposited gold films exhibiting high thermal stability when annealed in vacuum were reported. The aim of the present work is to provide more information on the origin of this phenomenon. The thermal stability of nanocrystalline gold films, made by advanced gas deposition, was investigated using in-situ four-probe electrical conductivity measurements. Four different samples, with different densities, were studied after annealing in vacuum at 473, 573, 673, and 773 K for 2 h. Films with low density displayed higher thermal density and weaker grain growth than dense films. The porous nanocrystalline films were stable up to at least 773 K. Scanning Electron Microscopy was applied to two of the samples, one with high density and one with low density, to analyse the morphology in the films after each annealing step. The activation energy for grain growth was decreased as the density was increased.

P3.39

SELF-ORGANIZATION IN NANOCRYSTALLINE GOLD FILMS DURING GAS DEPOSITION. P. Chaoguang, J. Ederth, L.B. Kish, J. Kopniczky, S. Zhao, C.G. Granqvist, Department of Materials Science, The Angstrom Laboratory, Uppsala University, Uppsala, SWEDEN; S.J. Savage, Department of Electromagnetic and Optic Materials, Swedish Defence Research Establishment, Linköping, SWEDEN.

In-situ electrical transport measurements were carried out in nanocrystalline gold films during inert gas deposition. The time dependence of the conductivity showed various self-organization phenomena, including aspects of: - biased percolation: conductor-insulator transition; - biased percolation: bad conductor-good conductor transition; - annealing; - sintering; - electromigration. The different effects were identified by recording the time-dependence of the conductance, by varying the deposition conditions, and by structural analysis.

P3.40

RHEED OBSERVATION OF TIN ATOMIC CHAINS FORMATION ON VICINAL GALLIUM ARSENIDE PLANE. Aleksey Senichkin, Aleksandr Bugaev, Vladimir Mokerov, Inst of Radio Engineering and Electronics of RAS, Moscow, RUSSIA.

Tin delta-doped GaAs structures grown on vicinal {001} GaAs surfaces by MBE method reveal the anisotropy of electrical conductivity and magneto-transport of electrons in directions along and across terrace edges of the vicinal plane [1]. These facts enable to suppose that the distribution of Sn dopant atoms in delta plane is un-uniform; namely - the tendency of the chains formation exists. In this work the direct observation of Sn atomic chains formation during-delta-deposition has been made. For this purpose the quantitative RHEED method of surface morphology characteristics determination by means of angular intensity distribution measurements was used. The optimal conditions for Sn atomic chains formation on GaAs vicinal surface oriented 3 degrees from the exact {001} orientation to {111} plane were determined for molecular beam epitaxy. It was established, that the chains formation depends on the structure of terraces of the initial vicinal plane before delta-deposition. It was shown that more than 70% of tin atoms may be in

the chain body, and the others 30% has uniform distribution on the terraces of the vicinal plane.

This work was supported by Scientific Program "Physics of Solids Nanostructures", Grant 97-2020.

[1] V.A. Kulbachinskii et. al. Microelectronic Engineering, v. 43-44 (1998), pp.319-324.

P3.41

FRAC TAL CHARACTERIZATION OF THE MORPHOLOGY OF CLUSTER-ASSEMBLED CARBON FILMS. Claudio Castelnovo, INFN - Università degli Studi di Milano, Dept of Physics, Milano, ITALY; Alessandro Podestà, INFN - Università di Milano-Bicocca, Dept of Materials Science, Milano, ITALY; Paolo Piseri, Emanuele Barborini, Paolo Milani, INFN - Università degli Studi di Milano, Dept of Physics, Milano, ITALY.

The morphology of nanostructured materials affects most of their physical and chemical properties. Cluster assembling of thin films has recently emerged as a promising technique for the fabrication of systems having a structure at the nanoscale. The ability to control the morphology of nanostructured films over different length scales is of paramount importance for the understanding of cluster assembling growth. Fractal analysis, describing scale invariance and spatial correlation of film surfaces, is particularly useful to this purpose. Using Atomic Force Microscopy (AFM), we have carried out a systematic morphological characterization of nanostructured carbon films grown by Supersonic Cluster Beam Deposition. We have investigated the dependence of film morphology on different cluster size distribution over a film thickness in a range from 100 nm up to 20 nm. We have recognized two different regimes in the film growth. At low thickness, clusters aggregate in mound-like basic units, whose size depends on precursors mass distribution but not on film thickness. Fractal analysis shows a correlation length comparable with the basic unit size. Over this length, the films are uniform and flat. At higher thickness, roughness increases and disordered isolated structures, much larger than the basic units, appear. Above a characteristic thickness, dependent on cluster precursor size, the onset of a cauliflower-like scale-invariant morphology is seen. Our results provide new insights on the mechanisms of growth of cluster-assembled systems.

P3.42

LOW-TEMPERATURE FORMATION OF CRYSTALLINE AND AMORPHOUS NANOSIZED ALUMINOSILICATE BY MINERALIZATION. Peter J. Stenhouse, Lynne A. Samuelson, Il-Young Kim, Materials Science Team, U.S. Army Natick Soldier Center, Natick, MA; Changmo Sung, Center for Advanced Materials, University of Massachusetts, Lowell, MA.

Crystalline and amorphous aluminosilicate particles were obtained at temperatures between 30°C and 50°C through the mineralization of aluminum alkoxides and silicon alkoxides onto multilayer polymer film templates. Crystal structure, phase identification, and morphology were characterized by energy dispersive x-ray spectroscopy (EDXS) and microdiffraction in transmission electron microscopy. The effects of temperature, concentration, and mineralization time on the structure of the resulting ceramics were studied. Crystalline mullite (3 Al₂O₃ * 2 SiO₂) was obtained when the molar ratio of Si to Al atoms exceeded 0.5. At higher relative concentrations of Al, amorphous Si-Al-O nanoparticles were obtained, with diameters on the order of 100 nm. In this presentation, optimized processing conditions are discussed along with possible explanations of the mechanisms of nanocrystalline formation.

P3.43

GROWTH BEHAVIOUR OF ENGINEERED POROUS THIN FILMS - MEASUREMENT AND MODELING. D. Vick, B. Dick, S.R. Kennedy, M.J. Brett, Dept. of Electrical and Computer Engineering, University of Alberta, Edmonton, Alberta, CANADA; T. Smy, Dept. of Electronics, Carleton University, Ottawa, Ontario, CANADA.

Recent experimental work has demonstrated that unique high porosity thin films may be obtained in physical deposition systems by combining glancing angle deposition with in situ substrate motion control. The microstructure of these films consists of isolated columns engineered into shapes such as helices, posts, or chevrons. Due to the isolated nature of the columns, the films present a unique opportunity to study fundamental thin film growth behaviour and, in particular, the influence of the self shadowing mechanism in three dimensions. Apart from this academic motivation, there is the need to characterize the physical constraints imposed on the engineering of these films. In particular, this study will have implications for the realization of isolated, periodically arranged nanostructures envisioned for certain applications. Results from an ongoing study of growth dynamics, morphology, porosity, and scaling behaviour, and the dependence of these features on deposition parameters, will be reported. Analysis of atomic force microscope and scanning electron microscope images will

be compared with predictions of the recently-developed three dimensional ballistic simulator 3D-FILMS.

P3.44

Abstract Withdrawn.

P3.45

GROWTH MORPHOLOGIES AND SURFACE ENHANCED RAMAN SCATTERING OF PLATED SILVER ON NANOPARTICLE SUBSTRATES. Joseph B. Jackson and Naomi J. Halas.

Electroless plating of nanoscale (5-20 nm) metal films onto functionalized silica nanoparticle substrates can produce core-shell nanoparticles with strongly geometry-dependent optical resonances, known as Metal Nanoshells. For silver deposition, the morphology of the metal layer can vary dramatically and is highly dependent on the reducing and stabilizing agents used for deposition. Film morphologies ranging from spiky to rough (reminiscent of aggregated clusters) to smooth on the 1-10 nm length scale were all observed and grown reproducibly. The observed variations in metal film morphology may provide insight into the role of reductant and stabilizer in the deposition kinetics of metals, particularly of nanometer scale thickness. Each film morphology gave rise to nanoparticles with unique optical signatures that could be analyzed via Mie scattering theory. Surface enhanced Raman Scattering was performed on paramercaptoaniline adsorbed onto the silver covered nanoparticles. Both plasmon-related and roughness-related local field enhancements contributed to SERS enhancement factors of over 10^6 using infrared (Nd:YAG) laser excitation.

P3.46

VAPOR PHASE HOMOEPITAXY OF GaAs ON (100) AND (100)/(111)A SURFACES. M.A. Nemirovskaya, R. Venkataramani, K.F. Jensen, Dept. of Chemical Engineering, MIT, Cambridge, MA.

GaAs substrates are widely used for building electrical and optical devices. While (100) surfaces are used most frequently, the deposition on patterned GaAs surfaces, such as grooved (100) surfaces, is currently of great interest. Grooves are formed by (111) surfaces and can be used for quantum wire or dot deposition. In the present work, we investigate physical processes involved in homoepitaxy of GaAs under VPE conditions on (100) surface and the evolution of (100)/(111)A edge using kinetic Monte Carlo techniques. The obtained results are compared with the available experimental data. To predict correctly the microscale evolution of (100) surface, such as growth mode transitions and island density, a model should incorporate both Ga and As atoms dynamics. Our study confirms the importance of self-surfactant effects for microstructure predictions on this surface. Also, we observe directly the evolution of (100)/(111)A edge. This evolution is largely determined by the relative rates of Ga diffusion on two different orientations and inter-diffusion. This work provides new information about individual processes occurring on GaAs surfaces during growth and their relative importance. It is also the first step into investigation of the deposition on complex patterned surfaces.

P3.47

MICROSTRUCTURE AND OPTICAL PROPERTIES OF CO SPUTTER DEPOSITED Si-Al NANOCOMPOSITE THIN FILMS. Feng Niu, Department of Materials Science and Engineering and Materials Research Center, Northwestern University, Evanston, IL; Peter J. Bobson and Brian Cantor, Oxford Centre for Advanced Materials and Composites, University of Oxford, Oxford, UNITED KINGDOM.

There has been increasing interest in developing novel nanocomposite thin film materials with potential in the opto-electronic device applications of the future. The metal-semiconductor nanocomposite thin films with small metal particles finely dispersed in a Si matrix, for example, are expected to have potential applications in the areas of optical selective filters, optical sensors and detectors, photo-conductors and thermionic emitters, due to enhanced surface plasma resonance absorption mode of nano-sized metal particles. Novel Si-Al composite thin films were grown by radio frequency co-sputtering of Si and Al with Al content in the range from 0 to 70 at.%. The microstructure and optical properties of the films were characterised by X-ray diffractometry, conventional and high-resolution transmission electron microscopy and spectrometry in the wavelength range from 200 to 3000 nm. Film microstructure was found to consist of nano-sized Al particles (< 10nm) embedded in an amorphous SiAl matrix. The optical absorption spectra of the films up to 50 at.% Al exhibited sharp absorption peaks below 500 nm and relatively low absorption above 500 nm. In addition, the absorption peaks shifted towards the longer wavelengths and total absorption above 500 nm increased remarkably as Al content increased. For the Si-69 at.% Al films, however, an absorption plateau appeared between 300 nm to 700 nm and a second weak and broad absorption peak appeared at

around 900 nm. The results are compared with the various effective medium theories, and it was found that the Sheng Ping theory with a modified dielectric function of bulk Al gives the best fitting to the measured optical spectra.

P3.48

SELF-ORGANIZATION AND TRANSROTATIONAL MICROSTRUCTURES FORMED DURING CRYSTALLIZATION OF THIN AMORPHOUS FILMS. Vladimir Yu. Kolosov, Ural State Economic Univ, Engineering Dept, Ekaterinburg, RUSSIA.

As we reported earlier [1] the crystal growth in thin amorphous films can be associated with an unusual phenomenon: strong (up to 100° per μm) regular dislocation independent rotation of the lattice round an axis (or axes) lying in the film plane. This internal lattice bending (transrotational microstructure) has been revealed and studied (mostly in situ, using transmission electron microscopy bend-contour technique [1]) for the films of different chemical bonding, prepared and crystallized by various methods: Se, Te, Sb_2Se_3 , Sb_2S_3 , Cu-Te, CuSe, Ge-Te, Fe_2O_3 , CoPd and some others. In the present paper we describe geometry, morphology, texture, gradients of lattice orientations, dynamics of crystal growth for the different kinds of self-organized microstructures which have complex variations in the crystal lattice orientation and imperfection but form regular patterns. Video of in situ transmission electron microscopy observations for the most complex microstructures (with target-like alternating circular zones formed in pyrolytic amorphous iron oxide films [2] with the help of electron beam annealing) is prepared. The dynamic changes of the diffraction contrast for the large growth rates (revealed by the analysis of the video) fit the proposed mechanism of the phenomenon based on the surface nucleation. Hypothetical atomistic model corresponding to the conformal transformation of usual crystal lattice is also proposed. [1]. V.Yu. Kolosov, Proc. XII ICEM, Seattle, 1, 574 (1990). [2]. V.Yu. Kolosov, A.R. Thölen, Acta Mat., 48, 1829 (2000).

P3.49

Abstract Withdrawn.

P3.50

MESOSCOPIC PATTERNING INDUCED BY CO-DEPOSITION OF C_{60} AND Ni ON THE $\text{MgO}(100)$ SINGLE CRYSTAL. Jiri Vacik, Hiroshi Naramoto, Kazumasa Narumi, Advanced Science Research Center, Japan Atomic Energy Research Institute, Takasaki, Gunma, JAPAN; Shunya Yamamoto, Dept of Materials Development, Japan Atomic Energy Research Institute, Takasaki, Gunma, JAPAN.

Spontaneous generation of complex ordered structures in inorganic systems is both arresting and potentially useful. It is apparent to single compounds, commixtures and alloys as well, and takes place in various spatio-temporal scales. Here we describe the self-arranged mesoscopic stripe structures formed during co-deposition of C_{60} and Ni on the $\text{MgO}(100)$ substrate. It was found that the periodic stripe systems could be grown if specific deposition kinetics (e.g. deposition rates of C_{60} and Ni < 0.1 nm/s, temperature of substrates $\sim 500^\circ\text{C}$, thickness of the Ni C_{60} adlayer ~ 100 nm) is applied. Several hierarchically grown self-organized assemblies were observed in the sample. The assemblies comprise hundreds of several mm long domains with thickness and spacing of 1 - 2 μm and height of about 1 μm . The stripes are anchored into a thin platform consisting of epitaxially grown Ni and a-C layers formed at the very beginning of the co-deposition process. The stripes are composed of sub-micron sized Ni particles surrounded by a polymerized NiC_{60} rind, and a-C structures identified between the stripes and on their hangs. As a possible mechanism of the distinct stripe formation a spatio-gradual relaxation of the accumulated stress in the phase-segregated Ni and C_{60} / a-C immiscible clusters is suggested. The periodic stripe system observed in the Ni C_{60} / $\text{MgO}(100)$ interface might find applications in optical devices, such as diffraction gratings and optical sensors.

P3.51

FORMATION AND OPTICAL CHARACTERISTICS OF SINGLE AND DOUBLE InAs SELF-ASSEMBLED QUANTUM DOTS. Cheol-Koo Hahn, Junichi Motohisa, Takashi Fukui, Research Center for Interface Quantum Electronics, Hokkaido Univ, Sapporo, JAPAN.

We report on the formation of position and number controlled InAs self-assembled quantum dots (SAQDs) and their optical characteristics. Single and double SAQD(s) were formed by selective area (SA) metal organic vapor phase epitaxy (MOVPE) on partially SiN_x masked GaAs (001) substrate. The mask layers were patterned to lines/spaces along the [110]-direction and somewhat wider rectangular openings attached to the lines. As a result of SA-growth pyramidal shaped GaAs structures were constructed at the rectangular regions of the pattern. A very narrow (001)-facet, in the range between 70 nm to 220 nm which is surrounded by {111}B and {110} sidewalls, was the top-facet of the pyramidal structures. Following InAs growth resulted in a number controlled SAQDs

formation only on the top of the narrow (001)-facets. Their size was in the range from 10 nm to 85 nm which could be determined by the InAs growth thickness. It was found that the interfacet adatom migrations and a great disparity of the growth rate between narrow (001)-facet and surrounding high Miller index surface plays an important role in the formation property of InAs SAQDs on narrow (001)-facet. The design parameters of the pattern such as mask opening ratio, adatom sink around pattern definition also affect the SAQDs formation. The number of the SAQDs formed on the (001)-facet was strongly dependent on the width of the top facet, so that the control of single- or double- SAQD(s) formation possible. Optical characteristics of position controlled single and double SAQD(s) were appraised by low temperature spatially resolved photoluminescence (PL) measurement. Narrow luminescence lines from the position controlled double SAQDs were detected at around 1.30 eV with a full width at half maximum (FWHM) of less than 0.5 meV. More details about the number and position control of SAQDs and their optical characteristics will be presented.

P3.52

OFF-AXIS EPITAXY IN A LATTICE MISMATCH SYSTEM. Akimasa Yamada, Paul J. Fons, Shigeru Niki, Hiroyuki Oyanagi, Electrotechnical Laboratory, Optoelectronics Division, Tsukuba, JAPAN.

Cu thin films were deposited on (001)-oriented GaAs substrates using molecular beam epitaxy (MBE). X-ray diffraction analysis proved that axis [100] of the Cu film laid in the substrate surface plane and parallel to the substrate [110] direction, while the [001] axis of the film was found to tilt predominantly in four directions at 7.20 degrees from the substrate surface normal. The tilt axes were oriented approximately parallel to the [100] and [010] directions of the substrate. The mechanism of tilt growth was modeled using an interface construction that leaves regions other than the interface of both materials free of strain. This consideration introduces a new type of defect which is formed periodically along the interface where an atomic step of the tilting film is encountered. The average interval between successive defects can be estimated using the lateral lattice spacing of both materials and the atomic step height of the film; the tilt angle can also be calculated geometrically. The calculated tilt angle agreed well with experiment, consistent with the model. Such tilt growth is not desirable as it results in the formation of multi-domains with different orientations. However, by using vicinal substrates, a method is proposed to grow a single domain film by using a substrate cut to an angle that allows an off-axis fit to the lattice plane of the film. In particular, the film must be grown with one of its principle axes perpendicular to the substrate surface crystallographic tilt. For off-axis growth the lattice strain concentrates at the interface and the remainder of the film is nearly stress free. The defect formation energy for off-axis growth becomes greater when the tilt angle is small in contrast to pseudomorphic growth. The critical lattice mismatch necessary for off-axis growth will also be discussed.

P3.53

Transferred to P2.6

P3.54

CONTINUUM SIMULATION OF ANISOTROPIC SURFACE EVOLUTION: ETCHING OF SILICON IN KOH. Markus Rauscher, Thierry Cretegnay, James P. Sethna, Cornell University, Department of Physics, LASSP, Ithaca, NY; Rikard A. Wind, Melissa A. Hines, Cornell University, Department of Chemistry, Ithaca, NY.

Chemical etching of silicon in KOH shows a strong dependence of the etch rate on the surface orientation. Recently developed experimental techniques allow to map out the angle dependence of the rates and the resulting surface morphologies systematically. The etch rates as a function of the surface orientation can be parametrized by a novel method specially designed to fit the cusps for the high symmetry surfaces (111), (110), and (100). In continuum simulations we model the etching of a silicon surface in KOH using finite difference schemes and level set methods to study the effect of the anisotropy of the etching rate on the surface morphology. The above described methods allow to run the simulations efficiently with the measured angle dependency of the etch rates. We describe the formation of facets, the coarsening dynamics, and the relationship to the experiments of Hines and Wind.

SESSION P4: MAGNETISM IN FILMS

Chair: Bene Poelsema
Tuesday Morning, November 28, 2000
Room 302 (Hynes)

8:30 AM P4.1

UNUSUAL MAGNETIC PROPERTIES OF Fe/Ni BILAYERS ON

Cu(100). Xiangdong Liu, Bernd Schirmer, Matthias Wuttig, RWTH, Aachen, GERMANY.

The epitaxial growth of fcc Fe/Ni bilayers has been studied using low energy and medium energy electron diffraction, (LEED and MEED, respectively). Pseudomorphic growth of up to 20 monolayer (ML) thick bilayers has been observed. Interesting enough, the Ni film has nevertheless a strong influence on the magnetic properties of the iron film. While the structural phases of the iron film resemble those found on Cu(100), the magnetic properties show strong deviations. In particular, evidence for a coupling of different ferromagnetic (FM) portions of the bilayer are found. This leads to an unusual temperature dependence of the magnetization for Fe film thicknesses between approximately 5 and 10 ML. The observation can be attributed to a ferromagnetic ordering at the Fe/Ni interface and a ferromagnetic ordering at the Fe film surface. The magnetic coupling does not only depend upon the Fe film thickness and temperature, but also the Ni film thickness. This behaviour is correlated with the film structure and morphology. For even thinner Fe films, exchange biasing is observed for a limited range of Fe film thicknesses. This unusual behaviour can be attributed to the structure of the Fe films and the magnetic coupling to the underlying Ni film.

8:45 AM *P4.2

GROWTH KINETICS AND MAGNETIC TRANSITIONS IN Fe/Cu(100). M.S. Altman, K.L. Man, Dept. of Physics, Hong Kong University of Science and Technology, HONG KONG; H. Poppa, NCEM, Lawrence Berkeley Lab, Berkeley, CA.

The magnetic properties of ultrathin ferromagnetic films depend strongly upon film microstructure and morphology. It has also been the aim of much work in recent years to gain control of thin film morphology and microstructure through the kinetics of the growth process. In this talk, low energy electron diffraction (LEED) and spin polarized low energy electron microscopy (SPLEEM) investigations will be described that reveal a new relationship between growth kinetics, microstructure and magnetism in Fe/Cu(100). By monitoring diffraction intensity oscillations and the evolution of magnetization simultaneously and continuously during growth with SPLEEM, magnetism and film thickness can be correlated with unprecedented precision. Using this approach, the generally accepted behavior of this system was reproduced in our work. However, the impact of deposition rate upon magnetic transitions in Fe/Cu(100) has been observed, including the onset of ferromagnetism and transition to the live layer phase at room temperature, and the Curie temperature of the live layer phase. Where possible, these results are confirmed by laterally averaging RHEED and MOKE measurements. LEED spot profile analysis rules out surface roughness as the cause of the observed phenomena. Instead, it will be shown how the effect of deposition rate on magnetic transitions in Fe/Cu(100) originates in details of interface formation and intermixing in the initial two Fe monolayers.

9:15 AM P4.3

RELAXATION OF THE ELASTIC STRAIN OF FePd GROWN ON Pd(001) AND FePt GROWN ON Pt(001) THIN FILMS. D. Halley, A. Marty, Y. Samson, J.P. Attane, P. Bayle, DRFMC/SP2M/NM, CEA Grenoble, FRANCE; B. Gilles, LTPCM-ENSEEG, St. Martin d'Heres, FRANCE.

The relaxation of strained epitaxial thin films in pure metals and semiconductors has been widely studied. However, relatively little work has been performed on strained layers consisting of metallic alloys. Nevertheless ordered magnetic alloys grown by molecular beam epitaxy (CoPt, FePd, FePt...) have been recently intensively studied for their magnetic properties, i.e large perpendicular magnetic anisotropy leading to high density recording technological developments. These ordered alloy layers are grown on various substrates or buffer layers (Pd, Pt, MgO...) to obtain the best state of chemical order needed to obtain large perpendicular anisotropy. Due to the misfit of the epilayer with respect to the substrate, relaxation defects may appear and affect the magnetic properties. In the molecular beam epitaxial growth of FePd on Pd(001) and FePt on Pt(001), we have shown by Transmission Electron Microscopy that the relaxation occurs mainly by the formation of microtwins. They are formed by the successive gliding of partial dislocations of Burger's vector $1/6\{1,1,2\}$ on the inclined planes (111). These defects lead to a linear steps at the surface of height, $n/3$ (in lattice units), aligned along the {110} in-plane directions. Here n is the number of partial dislocations involved in the formation of the defect. We have observed these steps by Near Field Microscopy for several thicknesses of the epilayer and we have performed a quantitative image analysis of the step height and step density distribution. These results will be interpreted in the framework of an elastic model of the relaxation. Then, the interplay between microtwins and magnetic properties will be presented.

9:45 AM *P4.4

MESOSCOPIC MAGNETS: DOTS, WIRES, AND PILLARS ON THE NANOMETER SCALE. J. Kirschner, Max-Planck-Institut fuer Mikrostrukturphysik, Halle, GERMANY.

Mesoscopic magnetic structures play an increasingly important role in magnetic storage technology, magnetic sensors, non-volatile random access memories, and "magneto-electronics" in general. Lithography-type processes for making such structures, though having been quite successful, will not be covered in this talk. Rather, typical surface science approaches, involving adsorption, surface diffusion, epitaxial growth phenomena, and self-organization will be exploited to produce and characterize mesoscopic magnetic structures. For example, magnetic wires may be made by step edge decoration on stepped single crystal surfaces by tuning surface diffusion. Likewise, magnetic dots may be created by exploiting localized adsorption on reconstructed surfaces. By repeated deposition of Co and Au in a controlled way, magnetic pillars with an aspect ratio of height: diameter of 2:1 with ~ 3 nm diameter may be grown. A particular challenging task is the magnetic characterization of such structures on the nanometer scale. Recent progress in spin-polarized tunneling with a magnetic tip is presented, with a lateral resolution of one nanometer at present.

10:15 AM P4.5

THE ROLE OF ATOMIC EXCHANGE IN THE INITIAL GROWTH OF CO ON Cu(001): A DFT-KMC STUDY. Rossitza Pentcheva, Matthias Scheffler, Fritz-Haber Institut der MPG, Berlin, GERMANY; Kristen Fichtorn, Department of Chemical Engineering, Pennsylvania State University, University Park, PA.

The the early stages of heteroepitaxial growth of Co on Cu(001) are studied with *ab initio* kinetic Monte Carlo (kMC) simulations, *i.e.* kMC with rates of the atomistic processes calculated by density-functional theory (DFT), employing the FP-LAPW method. DFT-calculations show that for low coverages Co adatoms prefer to adsorb substitutionally as opposed to adsorption at a fourfold hollow site. Due to the exchange processes substrate adatoms are generated on the surface. We find that the substitutionally adsorbed Co atoms act as *nucleation* centers both for on-surface Co and Cu adatoms, the effect being stronger for Co. Further, we focus on the adatom diffusion of both species (Co and Cu) on flat regions and along steps on the Cu(001) surface. In particular, the influence of magnetism on the diffusion barrier of Co is studied. The rates of the microscopic processes obtained with DFT are used as input parameters in a kinetic Monte-Carlo (kMC) simulation of the initial growth of Co on Cu(001). The surface morphology and the scaling properties of island density are compared to the homoepitaxial case (selfdiffusion of Cu on Cu(001)) and deviations from the predictions standard nucleation theory are discussed. The activation of atomic exchange processes gives rise to dramatic changes in surface morphology and island density. The DFT-kMC results provide explanation of the *bimodal* growth mode, recently observed in STM-experiments (Nouvertné, *et al.*, Phys. Rev. B **60**, 14382 (1999)) and characterized by a high density of small Co-islands and large, Co-decorated Cu islands.

10:30 AM P4.6

PROBING THE SPIN PHASE DIAGRAM OF FCC Fe ULTRATHIN FILMS USING Co ATOMS. John Pierce, Maria Torija, Jian Shen, Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN.

Several ultrathin magnetic film systems exhibit a reorientation of magnetization as the film thickness is increased beyond some critical value. In some metastable systems, purely thickness driven spin reorientation is unfortunately masked by structural transitions. We present a method in which the magneto-optic Kerr effect (MOKE) can be used to uncover the "true" critical thickness (the transition thickness in the absence of structural changes) and anisotropy constants of a metastable film as a function of temperature. We demonstrate this method on the face-centered tetragonal (fct) Fe/Cu(100) system, which undergoes a structural transition to a face-centered cubic (fcc) phase at a thickness of 4 ML. Under ultra-high vacuum and at given temperatures, we evaporated small fractions of a monolayer of Co on fct Fe/Cu(100) films of various thicknesses. For each Fe film we determined the thickness of cobalt necessary to reorient magnetization from the direction perpendicular to the film to the in-plane direction. These experiments yielded a plot of Co critical thickness vs. Fe thickness at each temperature. The x intercept of these plots, the Fe thickness at which the spin would reorient without a Co capping layer, was taken to be the critical thickness for the fct Fe film. Our data directly results in a magnetic phase diagram for fct Fe films, which maps the magnetic state (magnetization perpendicular, or in-plane) in the space of temperature and Fe thickness.

10:45 AM P4.7

TUNABLE MAGNETIC PROPERTIES OF NANOSCALE MAGNETIC DOTS IN CERAMIC MATRIX. D. Kumar¹, J.

Narayan², A.K. Sharma², A. Kvit², C. Jin² and J. Sankar¹. ¹Center for Advanced Materials and Smart Structures, North Carolina A&T State University, Greensboro, NC; ²Department of MS&E, North Carolina State University, Raleigh, NC.

We have developed a novel thin film processing method based upon pulsed laser deposition to process nanocrystalline magnetic materials with accurate size and interface control. Using this method, single domain nanocrystalline Fe and Ni particles in 5-10 nm size range embedded in amorphous as well as crystalline alumina have been produced. Hysteresis below blocking temperature have been found to be consistent with the Stoner-Wohlfarth type behavior. The size of Fe and Ni nanodots measured using transmission electron microscopy and calculated using magnetic data are in excellent agreement with each other.

11:00 AM *P4.8

QUANTUM MIRAGES. H.C. Manoharan, C.P. Lutz, D.M. Eigler, IBM Research Division, Almaden Research Center, San Jose, CA.

While the correlated electron physics underlying the diverse manifestations of magnetism and spin have long been studied via macroscopic behavior, only recently have novel local probes opened the door to a new class of studies on the nanometer length scale. On top of these technological advances, the advent of controlled atomic and molecular manipulation provides a unique opportunity not only to detect spin phenomena at atomic length scales, but to manipulate spins as well. This talk will detail new results¹ that exploit these techniques using low-temperature scanning tunneling microscopy. We have directly imaged the electronic perturbation arising from the spin-compensation cloud formed around isolated magnetic moments on a metal surface. Utilizing the detection of this many-body state—known as the Kondo resonance—in a type of teleportation experiment, we demonstrate that the spectroscopic signature of an atom may be sampled and projected to a remote location by means of a surrounding two-dimensional electron gas confined in an engineered nanostructure. The "quantum mirage" thus cast by a single magnetic atom can be coherently refocused at a distinct point where it is detected as a phantom atom around which the electronic structure mimics that at the real atom. Once materialized, this phantom can interact with real matter in intriguing ways. We have also been developing a novel communication method based on this effect. 1. H.C. Manoharan *et al.*, Nature **403**, 512 (2000).

11:30 AM P4.9

ULTRAFAST MAGNETIZATION REVERSAL DYNAMICS ON A MICROMETER-SCALE THIN FILM ELEMENT STUDIED BY TIME DOMAIN IMAGING. B.C. Choi, G. Ballentine, M. Belov, W.K. Hiebert, M.R. Freeman, University of Alberta, Dept of Physics, Edmonton, AB, CANADA.

Picosecond time scale magnetization reversal dynamics in a 15 nm thick Ni₈₀Fe₂₀ microstructure (10 μ m \times 2 μ m) is studied using time-resolved stroboscopic scanning Kerr microscopy and micromagnetic simulations. The time domain images reveal in detail a striking change in the magnetization reversal mode, associated with the dramatic reduction in switching time when the magnetization vector is pulsed by a longitudinal switching field while a steady transverse biasing field is applied to the sample. According to the time domain imaging results, the abrupt change of the switching time is due to the change in the magnetization reversal mode; *i.e.*, the nucleation dominant reversal process is replaced by domain wall motion if transverse biasing field is applied. Furthermore, magnetization oscillations subsequent to reversal are observed at two distinct resonance frequencies, which sensitively depend on the biasing field strength. The high frequency resonance at $f=2$ GHz is caused by damped precession of the magnetization vector, whereas another mode at $f\approx 0.56$ GHz is observed to arise from domain wall oscillation.

SESSION P5: THIN FILM NUCLEATION, GROWTH AND ALLOY FORMATION

Chair: John A. Venables
Tuesday Afternoon, November 28, 2000
Room 302 (Hynes)

1:30 PM *P5.1

KINETIC EFFECTS IN EPITAXIAL GROWTH. J. Tersoff, IBM T.J. Watson Research Center, Yorktown Heights, NY.

Epitaxial growth is controlled by an interplay between thermodynamic and kinetic driving forces. The role of kinetics is especially obvious in unstable systems, or in growth far from equilibrium; but even the smoothing of unstrained surfaces during annealing can be far more complex than a simple relaxation toward equilibrium. This talk will review some kinetic effects that can

dramatically influence morphology and alloy composition, but that have been to some extent either neglected or incompletely understood. These include the effects of surface segregation, differences in atomic mobility between alloy components, and adatom attachment barriers within the classic continuum picture of growth.

2:00 PM **P5.2**

LEVEL SETS REVERSIBLE ISLAND GROWTH. Max Petersen^{1,2}, Christian Ratsch^{2,3}, Russel Cafisch², Mark Gyure³ and Andrew Zangwill¹. ¹Georgia Tech, School of Physics, Atlanta, GA; ²UCLA, Dept. of Mathematics, Los Angeles, CA; ³HRL, Malibu, CA.

The level set approach applied to the modeling of epitaxial growth allows a description which is discrete (atomistic) in the height profile and continuous in the lateral dimensions. Therefore, virtues of continuum and discrete models can be combined. The feasibility of this approach in the case of homoepitaxial growth with irreversible aggregation has been successfully shown [1]. In this model, island boundaries evolve with a velocity that is obtained by solving the diffusion equation. Here we present an extension to the island dynamics model to include reversibility, i.e., the possibility of thermal detachment of atoms from island edges. As a consequence, islands do not always grow, and break-up of islands is explicitly allowed in our approach. We make no assumptions about a critical nucleus. A qualitative and quantitative comparison of island densities and island size distributions to those obtained from kinetic Monte Carlo simulations will be given.

[1] C. Ratsch, S. Chen, M. Kang, M.F. Gyure, and D.D. Vvedensky, Phys. Rev. B **61**, R10598 (2000).

2:15 PM **P5.3**

SIMULATIONS OF MOLECULAR BEAM EPITAXY GROWTH OF GaAs. Brad G. Orr, Zili Zhang, Department of Physics, University of Michigan, Ann Arbor, MI.

Molecular beam epitaxy (MBE) growth has been numerically modeled for many years by a number of practitioners. In this talk we will present a "minimal" model for the growth of these compounds. The key aspects of the simulation include two deposited species one volatile and the second with high surface mobility. Simulations reproduce the experimentally observed adatom concentrations for GaAs and show that smooth surfaces are produced for films deposited with a substrate temperature in a crossover regime between kinetically limited and entropically roughened growth. We will also compare our numerical results with recently published work on specular ion scattering from growing films. The surface dynamics produced by our growth simulation are quite different from those produced by single component models. We will discuss some of the strengths and weaknesses of studying such a highly idealized model for MBE growth.

2:30 PM **P5.4**

THE EHRLICH-SCHWOEBEL EFFECT FOR VACANCIES: LOW-INDEX FACES OF SILVER. Michael I. Haftel, Naval Research Laboratory, Washington, DC.

We employ surface-embedded-atom-method potentials to investigate the diffusion barriers of vacancies diffusing over and near steps on the low index faces of silver. Barriers for vacancy terrace diffusion, diffusion over step-edges, and diffusion along step edges, including around kinks and corners, are calculated and systematized according to coordination and bond breaking. Vacancies are significantly less mobile than adatoms and have large Ehrlich-Schwoebel (ES) barriers on all three faces. For Ag(100) the diffusion barrier for vacancies along step-edges is virtually the same (474 meV) as on the terrace. As in diffusion near the step edge, vacancies encounter a significant increase (213 meV) in the activation barrier when diffusing around the corner of a vacancy island (the corner analogue of the ES barrier), but the excess barrier around a kink all but disappears because exchange diffusion is favorable there. The consequences of the vacancy ES effect on vacancy island shapes and 3D pitting are discussed and contrasted with the usual ES effects on adatom islands.

2:45 PM **P5.5**

ELEMENTAL PROCESS OF SURFACE SELF-DIFFUSION ON GOLD (001) SURFACE. Masao Doyama, T. Ohmae, Y. Kogure, Teikyo University of Science and Technology, Uenohara, Yamanashi, JAPAN.

Epitaxial growth of vapor deposition on (111) and (001) surfaces has been studied by use of molecular dynamics and Monte Carlo method. The activation energies and jump frequencies have been calculated by molecular dynamics using embedded atom potential at any temperatures. For example the activation energies for the motion of ad-atom clusters on (001) plane of gold are calculated. It was found that the activation energy of the motion of an ad-atom on (001) of gold is 0.63 eV. The activation energies of the dissociation in the direction of a di-adatom is 1.00 eV, and 0.63eV from the first to the

second nearest neighbor. The conversion energies of ad-atom clusters have been calculated. These were more than nearly half of one electron volt and much higher than those corresponding motion on (111) planes. The motion and growth of simulation will be shown using movies at various temperatures. A naming of ad-atom clusters is proposed.

3:30 PM ***P5.6**

ADSORBATE EFFECTS ON THIN FILM EVOLUTION: OXYGEN Ag/Ag(100). A.R. Layson, J.W. Evans, P.A. Thiel, Iowa State University, Departments of Chemistry and Mathematics, Ames, IA.

We have studied the effects of oxygen on the formation, structure, and post-deposition evolution of homoepitaxial films on Ag(100) by comparison to our previous studies of the same aspects of clean films [1]. High-resolution LEED and variable-temperature STM experiments show that oxygen does not affect film structure formed during deposition (e.g., island densities), but that evolution subsequent to deposition is accelerated strongly. This is true for coarsening of islands at submonolayer coverages, and for smoothing of rough films at multilayer coverages. By varying the sample temperature, and also the interaction of the sample with the electron beam, we can show that the acceleration of coarsening is an effect of atomic, not molecular, adsorbed oxygen. For the clean surface, our previous STM experiments had shown that the predominant mechanism of submonolayer coarsening was island diffusion and subsequent coalescence (Smoluchowski ripening). STM reveals now that oxygen changes this situation, making Ostwald ripening the most significant pathway. Quantitative analysis of STM images shows that reshaping processes are also accelerated markedly by adsorbed oxygen. [1] P.A. Thiel and J.W. Evans, J. Phys. Chem. B **104** (2000) 1663 (review article).

4:00 PM **P5.7**

KINETICS OF ALLOYING AT SURFACES: THE MECHANISM OF BRONZE FORMATION BY Sn DEPOSITION ONTO Cu(111). Andreas K. Schmid, Norm C. Bartelt, and Robert Q. Hwang, Sandia National Laboratories, Livermore, CA.

When Sn is deposited on top of Cu(111) it exchanges into the surface to form a surface bronze alloy. Using low-energy electron microscopy (LEEM) and scanning tunneling microscopy (STM) we find that the alloying proceeds via an extraordinarily interesting mechanism. During room temperature physical vapor deposition of Sn on Cu(111), similar to what one often observes in other cases of metal-on-metal epitaxy, the Sn quickly coalesces into 2D tin islands. Immediately after the formation of the Sn islands, however, a striking and unexpected motion sets in. Islands comprised of some 100,000 atoms roam across the Cu surface, slowly shrinking in size until they disappear. We show how the islands are propelled by a surface bronze formation reaction occurring at the interface between the islands and the Cu crystal. This dance of the Sn islands might be thought of as rather exotic. However it arises naturally out of two simple atomic facts. Sn exchanges into Cu much more slowly than Sn diffuses on top of Cu, and Sn is repelled by already incorporated Sn. So this complex alloying reaction might not be at all rare, and indicates that even very simple atomic mechanisms can lead to surprisingly curious phenomena on the mesoscopic scale. This work was supported by the Office of Basic Energy Sciences of the US DOE under contract no. DE-AC04-94AL85000

4:15 PM **P5.8**

STRAIN-INDUCED PHASE SEGREGATION IN SUBMONOLAYER Ag-Co ALLOY FILMS ON Ru(0001). G.E. Thayer, UC Davis; V. Ozolinš, A.K. Schmid, N.C. Bartelt, J.J. Hoyt, R.Q. Hwang, Sandia National Laboratories, Livermore, CA; M. Asta, Northwestern Univ., Evanston, IL; S. Chiang, UC Davis.

Using scanning tunneling microscopy (STM) and first-principles density-functional-theory calculations to study submonolayer films of Ag-Co surface alloys on Ru(0001), we have discovered a novel phase segregation mechanism. Competition between surface alloying and dislocation formation to relieve film/substrate mismatch strain leads to coexistence of a pseudomorphic Co-Ag surface alloy phase and a dislocated pure Ag phase. Atomically resolved STM images of the Co-Ag surface alloy phase exhibit disordered nanoscale droplets of pure Ag in a matrix of pure Co, in good agreement with the results of our first-principles calculations.

4:30 PM **P5.9**

A TWO-COMPONENT FRENKEL-KONTOROVA MODEL FOR SURFACE ALLOY FORMATION. István Daruka, John C. Hamilton, Sandia National Labs, Livermore, CA.

It has been shown by recent experiments that bulk immiscible metals (eg. Ag/Cu, Ag/Co, and Au/Ni) can form binary alloys on certain surfaces where the substrate mediates the elastic misfits between the

two components, thus relieving the elastic strain in the overlayer. These novel surface alloys exhibit a rich phase structure. We formulate a two-component Frenkel-Kontorova model in one dimension to study surface alloy formation. This model can naturally incorporate dislocation formation that plays a crucial role in determining the actual structure of the system. Using energy minimization calculations and Monte Carlo simulations we provide a phase diagram in terms of average alloy composition and the energy of mixing. Other related phenomena, like dislocation decoration and dislocation-dislocation interaction will also be discussed.

4:45 PM P5.10

SURFACE STRUCTURE AND METAL EPITAXY: Ag/Cu(111). Kenji Umezawa, Shigemitsu Nakanishi, Osaka Prefecture Univ, Dept. of Materials Sciences, Osaka, JAPAN; W.M. Gibson, The Univ of Albany at SUNY, Dept. of Physics, Albany, NY.

The growth mode of multi-layers of Ag atoms on Cu(111) has been investigated over a wide temperature range from 170K through 640K by using TOF-impact collision ion beam scattering spectroscopy. We found that two types of epitaxial growth exist: parallel and antiparallel orientation with respect to the Cu substrate. At substrate temperatures over 300 K. Moreover, the relative amounts of these two growth modes show an observed oscillatory dependence on the growth temperatures during Ag deposition. Measurements show that first-layer Cu atoms were shifted and localized in defined areas in which the stacking changed from ABC to ABA (hcp-sites).

SESSION P6: POSTER SESSION
THIN FILMS – MOSTLY INSULATING, ORGANIC,
DIAMOND, AND CVD/PVD GROWTH
Chair: Andreas K. Schmid
Tuesday Evening, November 28, 2000
8:00 PM
Exhibition Hall D (Hynes)

P6.1

INVESTIGATING THE EFFECT OF THE β -CR₂N TO CUBIC-CR_xN_y PHASE TRANSITION ON STRESS STATE IN CHROMIUM NITRIDE THIN FILMS. B.A. Rainey, S.M. Yalisove and J.C. Bilello, Center for Nanomaterials Science, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI.

Several series of chromium nitride thin films were deposited by reactive sputtering in two specific geometries. A series consisted of films with phase compositions varying from β - [hexagonal structure] Cr₂N to cubic [NaCl structure] Cr_xN_y ($x \geq .5, y = 1 - x$) or a mixture of the two phases. Nitrogen flow rate was systematically altered to produce the different phases. This was done to study the influence of the phase transformation of β -Cr₂N to cubic-Cr_xN_y on film stress state. The film stress within the plane of growth (in-plane) was calculated from lattice curvature measurements obtained with double crystal diffraction topography (DCDT). X-ray diffraction was used to characterize the phases of the films. DCDT analysis of films grown in one of the geometries shows that stress state changes from tensile to compressive as a function of increasing nitrogen flow. Phase analysis reveals that this trend coincides with the β -Cr₂N to cubic-Cr_xN_y transformation. However, a transition in stress state is not observed in conjunction the phase transformation in films grown in the other deposition geometry used in this study. We conclude that the tensile to compressive stress transition is nonindicative of a phase transformation. Results of this study indicate that the phase transformation promotes a decrease in tensile stress whereas other factors contribute to the production of compressive stress in these films.

P6.2

STUDY OF SILICON OXYNITRIDE FILMS PRODUCED BY RADIO-FREQUENCY PLASMA ASSISTED ELECTRON CYCLOTRON RESONANCE. Jason Brewer, Avi Raveh, Eugene A. Irene, Dept of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC.

New techniques for the development of higher dielectric constant materials as a passivation layer of silicon remains a challenge. In this study we used a radio frequency (RF) plasma process with and without an electron cyclotron resonance (ECR) plasma at low pressure and low temperature, in order to incorporate nitrogen into the grown layer. The combination of ECR with the RF plasma may reduce the damage in the passivation layer by lowering the ion energy. The layer was fabricated with an ECR power of 300 W and with the RF bias voltage (V_{rf}) in the range of 0 to -80 V. A low substrate temperature range of 100 to 300°C was used. The effect of the plasma processing variables on the structure, morphology, and composition of

the fabricated layers was studied by spectroscopic ellipsometry, Auger electron spectroscopy, and capacitance-voltage measurements. The maximum nitrided layer thickness was observed at a N₂:O₂ ratio of 1 and $V_{rf} = -50$ V. The nitride to oxide ratio in the grown layer was found to be dependent on the competitive processes between the O⁻ and N⁺ species. At $V_{rf} < -20$ V, a predominantly oxide layer was formed due to the relatively high concentration of O⁻, while at $V_{rf} > -50$ V the formation of the film proceeds mainly by NO and N⁺ ions and radicals. The effects of N₂:O₂ ratio, gas pressure, and V_{rf} on the composition and properties of the fabricated films are presented.

P6.3

GROWTH OF EPITAXIAL Al₂O₃ FILMS ON SILICON BY IONIZED BEAM DEPOSITION. SangWoo Whangbo, YunKi Choi, HongKyu Jang, ChungNam Whang, Yonsei Univ, Atomic-Scale Surface Science Research Center & Institute of Physics and Applied Physics, Seoul, KOREA.

Epitaxial Al₂O₃ films have been successfully grown on silicon substrate by the ionized beam deposition using Al ion beam in oxygen environment. The crystalline quality dependence of the Al₂O₃ films on the growth temperatures was investigated. Using *in situ* reflection high energy electron diffraction, the orientation relationships between epitaxial Al₂O₃ films and Si substrate were found to be (100) Al₂O₃//(100) Si with [1 $\bar{1}$ 0] Al₂O₃//[1 $\bar{1}$ 0] Si and (111) Al₂O₃//(111) Si with [1 $\bar{1}$ $\bar{2}$] Al₂O₃//[1 $\bar{1}$ $\bar{2}$] Si. The stoichiometry of the films was found to be similar to that of sapphire from XPS measurements.

P6.4

AN XPS STUDY OF THE EARLY OXYNITRIDATION STAGES OF IDEALLY HYDROGEN-TERMINATED (100) SILICON IN N₂O AMBIENT. G.F. Cerofolini, M. Camalleri, S. Lorenti, L. Renna, O. Viscuso, STMicroelectronics, ITALY; G.G. Condorelli, I.L. Fragala, Dept of Chemistry, Univ of Catania, ITALY.

The kinetics of oxynitridation of single crystalline silicon in the monolayer regime have been studied via high resolution x-ray photoelectron spectroscopy. The considered regime has forced us to prepare the surface with negligible oxygen defects; this was achieved by treating the surface in H₂ at temperature around 800°C. The oxidation kinetics were determined by using the 2p signal of bulk silicon as internal standard. Using a two-level (2s and 2p) method able to cancel the Madelung potential and relaxation effects, the charge transfer associated with the oxidation was also determined.

P6.5

NANO-SCALE HETEROEPITAXY CONTROL OF MAGNETIC OXIDE THIN FILMS ON ULTRA-SMOOTH SAPPHIRE SUBSTRATES. M. Takakura, J. Tashiro, T. Miyahara, M. Furusawa, M. Yoshimoto, Tokyo Inst. of Tech., Materials & Structures Lab., Yokohama, JAPAN.

From the point of application of ultra-high density magnetic memory devices and the search of new functional materials, we have examined the heteroepitaxy of magnetic oxide films for construction of low-dimensional structure. Here we report the formation of nanowires and nanodots of (Mn,Zn) ferrite, Fe₃O₄ as ferrite materials and NiO as an antiferromagnetic material. These films were deposited on ultra-smooth sapphire (0001) substrates (single-crystal aluminum oxide) by pulsed laser molecular beam epitaxy method (Laser MBE) coupled with reflection high energy electron diffraction (RHEED). Ultra-smooth sapphire (0001) substrates annealed in air at 1000°C have a surface state of stairs with step height of 0.2nm and terrace width of 100nm to 150nm. It is expected for atomic-scale flatness of substrates to enhance the epitaxial growth of the films and also step-flow growth when the temperature is high enough for precursors to migrate to the step edges leading to formation of the nanowires and nanodots. In case of the (Mn,Zn) ferrite, thick films were grown epitaxially in the spiral growth mode, but ultra-thin films became nanowires (0.5nm high, 20nm wide) along the atomic step edges. The height of 0.5nm for nanowires is close to an interplanar spacing of (Mn,Zn) ferrite (111) plane. By controlling the step height and terrace width of ultra-smooth substrates, the novel heteroepitaxy could be attained towards construction of low-dimensional structure.

P6.6

ON THE NUCLEATION MECHANISM OF cBN ON AN hBN BASELAYER. Jian Ye and Hans Oechsner, Center for Materials Research and Institute for Surface and Thin Film Analysis, University of Kaiserslautern, Kaiserslautern, GERMANY.

The growth of cBN layers by r.f. magnetron sputter deposition on Si (100) has been studied in dependence of the r.f. substrate bias voltage and the substrate temperature using Ar and N₂ as working gases. In particular, the time dependent evolution of the film thickness, i.e. the growth rate, and the films' surface roughness have been followed under continuous deposition. Quite surprisingly, a shrinking by about 30 nm

occurs when film thicknesses around 100 nm had been reached. When interrupting the deposition process before, during and after the period of negative growth rate, AFM images revealed the appearance of an increased surface roughness during the shrinking process. After the shrinking interval pure cBN growth was identified with Auger electron spectroscopy AES and low energy electron loss spectroscopy EELS. Sputter depth profiles with AES and EELS down to the substrates revealed the well known existence of a hBN base layer below the cBN region. The observed shrinking by almost 1/3 of the original film thickness indicates clearly a spontaneous phase transformation into sp^3 -coordinated cBN within the hBN bulk. The transformation depths is far above the range of about 1 nm of the Ar or nitrogen ions bombarding the growing film during deposition. The increased surface roughness during the shrinking process leads to the conclusion that at first cBN- grains develop locally in the initial hBN layer. The film surface becomes smooth again as soon as the grains have grown together to a complete cBN coverage. Based on the present results we propose a nucleation model which considers the minimization of the total film energy. According to this model a spontaneous nucleation occurs when the squared strain energy of the initial hBN layer exceeds that of a cBN film of equal mass but reduced thickness.

P6.7

GROWTH OF AlN AND TiN STRUCTURES BY PLASMA-ENHANCED PULSED LASER DEPOSITION. Edward Poindexter, Florida A&M University and the Florida State University, Dept. of Electrical and Computer Engineering, Tallahassee, FL; Yan Xin, National High Magnetic Field Laboratory, Tallahassee, FL; Steven M. Durbin, University of Canterbury, Dept. of Electrical & Electronic Engineering, Christchurch, NEW ZEALAND.

The pulsed laser deposition technique has been successfully applied to the growth of a wide range of materials, and is routinely used to fabricate high-quality oxide thin films. Growth of nitride-based materials, however, can be more difficult due to the large (~ 9.9 eV) binding energy of molecular nitrogen. This paper describes the growth and characterization of AlN and TiN structures grown by plasma-enhanced pulsed laser deposition. An aluminum target was ablated using a KrF excimer laser ($\lambda = 248$ nm) at various laser fluences, and active nitrogen species were obtained using an inductively-coupled RF plasma source. AlN films grown directly on bare (001) silicon or (0001) sapphire substrates were found to be either polycrystalline or amorphous depending on substrate temperature. In-situ RHEED indicated that single-crystal TiN films were obtained on both types of substrates, however, over the temperature range of investigated (500 - 800°C). AlN films deposited on a ~ 200 Å thick TiN buffer layer on silicon were found to be polycrystalline. In contrast, a ~ 600 Å thick single-crystal AlN layer was grown on a (0001) sapphire substrate by using a ~ 240 Å thick TiN buffer layer. TEM analysis shows that the defects most prevalent within the layer are threading dislocations. The interfaces of AlN/TiN and TiN/sapphire substrate are atomically smooth with only one or two monolayer roughness. The epitaxial relationship of the film to the substrate is $[0001]AlN//[111]TiN//[0001]sapphire$ along the growth direction, and the in-plane orientation consists of $[11\bar{2}0]AlN//[11\bar{2}]TiN//[11\bar{2}0]sapphire$, and $[\bar{1}100]AlN//[\bar{1}10]TiN//[\bar{1}100]sapphire$. Measured from the selected area diffraction pattern, most of the misfit strain between AlN/TiN, and TiN/sapphire (9% mismatch) is relieved.

P6.8

KINETICS OF HYDROTHERMAL GROWTH OF BaTiO₃ ON TiO₂ SINGLE CRYSTAL SURFACES. Victor Fuenzalida and Judit Lisoni^a, Universidad de Chile, Departamento de Física, Santiago, CHILE. ^aPresent Address: CSIC, Madrid, SPAIN.

TiO₂ (rutile) single crystal plates, with (001) and (110) orientation, were immersed in an aqueous solution of Ba(OH)₂ 0.5 M at temperatures of 100 and 150°C for 1 and 4 hours in order to grow BaTiO₃. SEM micrographs on the samples fabricated on the (001) surface displayed isolated grains with an average height ranging from 200 nm at 100°C to 700 nm at 150°C. On the other hand, samples with (001) orientation exhibited no growth at 100°C, and only a few grains along lines attributed to the polishing process of the substrate at 150°C. The image of backscattered electrons indicated that barium is concentrated on the grains in all cases. Only the (001) samples exhibited reflections of cubic BaTiO₃ by x-ray diffraction, as well as distinct Ba signals under x-ray photoelectron spectrometry. These results agree with the hypothesis of a dissolution-precipitation growth mechanism, in which dissolution is possible for the (001) face, but not for the (110) one, which is the most stable of the low-index faces of this material.

P6.9

AMORPHOUS VERSUS CRYSTALLINE DIELECTRIC FILMS: DIRECT DEMONSTRATION OF THIN FILM - SUBSTRATE ELECTRICAL INTERACTION. Igor Lubomirsky, Weizmann

Institute of Science, Rehovot, ISRAEL; Tzu You Wang and Oscar Stafsudd, Electrical Eng. Dept., UCLA, CA.

Electric properties of thin ferroelectric and dielectric crystalline films exhibit strong dependence on the film thickness and a nature of the substrate. At the same time, properties of thin amorphous films (SiO₂, Si₃N₄, glass etc.) do not show any substrate or thickness dependence. To identify the phenomenon characteristic for all dielectric films, it seems attractive to examine film - substrate interaction on a model system of thin non-ferroelectric films that have an identical chemical composition, but a different structure. We compared optical and dielectric properties of crystalline and amorphous Al₂O₃ films, both substrate supported and freestanding. The films were prepared by complete oxidation of aluminum metal layer deposited on (100) and (111) Si, followed by annealing at 700°C. The average thickness of aluminum oxide was 180 ± 4 nm irrespective of the film and substrate crystal structure. The refractive index of the crystalline films ($n=1.83-1.89$) was higher than that of the amorphous film ($n=1.76-1.785$) and much higher than those of the bulk sapphire ($n=1.69-1.71$). The dielectric constants, measured at 1 MHz, are 1.63 and 3.45 for crystalline and amorphous films respectively, which is much less than the value of a bulk Al₂O₃ (9-12). Measurements of Si wafer curvature prior and after oxide deposition revealed that both films are stress free. Surface Photovoltage measurements showed ≈ 350 mV band bending at the film-substrate interface, which implies that the substrate supported films are permanently subjected to a few tens kV/cm electric field. After the Si substrate was locally removed, leaving the films freestanding, neither amorphous nor crystalline films changed their thickness. However, the crystalline films show a decrease of refractive index (1.72-1.75) and an almost 6-fold increase (!) in dielectric constant (9.1-9.6), whereas the amorphous films showed no change. Because both amorphous and crystalline films were mechanical stress free and have the same chemical composition, the electrical interaction is responsible for the observed behavior. It also demonstrates that the thin film-substrate electrical interaction and polarization mechanisms are fundamentally different for crystalline and amorphous thin films.

P6.10

Transferred to P9.2

P6.11

MICROSTRUCTURE AND ELECTRICAL PROPERTIES OF INTERMEDIATE ZIRCONIUM LAYERS FOR MEDIUM-K DIELECTRIC APPLICATIONS. Nabil Bassim, Valentin Craciun, Joshua Howard, George Koval, Rajiv Singh, University of Florida, Dept of Materials Science & Engineering.

The development of high-K dielectric materials to replace the SiO₂ as the gate oxide in silicon-based MOS device structures has attracted much interest recently. One of the key challenges in producing oxide thin films has been to prevent the formation of an interfacial layer of SiO₂ between the film and the substrate, which subsequently reduces the effective gate oxide capacitance. One possible solution to this problem is the deposition of an intermediate layer that is more stable with the substrate than SiO₂. A thermodynamic argument can be proposed for the deposition of an intermediate zirconium layer which, when annealed in an oxygen ambient, can form a very thin zirconium silicate layer upon which a medium or high-K capping layer can be deposited. Thin (~ 15 Å) zirconium layers were deposited using pulsed laser deposition techniques and annealed in an oxygen atmosphere to form a stable zirconium silicate layer and ZrO₂ films were subsequently deposited in order to raise the K value of the structure. Cross-sectional high-resolution transmission electron microscopy and X-ray photoelectron spectroscopy were used to investigate the layers formed in this composite structure and the microstructure and processing parameters were related to the measured Capacitance-Voltage and Current-Voltage characteristics of the film.

P6.12

A SYNCHROTRON X-RAY SCATTERING STUDY ON OXIDATION OF EPITAXIAL AlN/Si(111). Hyun Chol Kang, Jin Woo Kim, Min Ho Kim, Seong Ju Park, Do Young Noh, Kwangju Inst of Science and Technology, Dept of MS&E, Kwangju, KOREA.

Thermal oxidation of epitaxial AlN(002)/Si(111) thin film was investigated in a synchrotron x-ray scattering experiment. As the annealing temperature was slowly increased to 600°C with the heating rate of 25°C/min, the nitrogen in the AlN was decomposed and the films became porous gradually. As the annealing temperature was increased to 750°C, a monoclinic θ -Al₂O₃ phase was formed, which is different from oxidation of epitaxial AlN/Sapphire films that are transformed into epitaxial cubic γ -Al₂O₃ phase. The hexagonal α -Al₂O₃ and cubic γ -Al₂O₃ phases are formed at a higher annealing temperature of $\sim 820^\circ\text{C}$. The AlN films rapidly annealed to 800, 900, 1000°C (heating rate of 350°C/min) are transformed into cubic γ -Al₂O₃ films that are epitaxial to the Si(111) substrate, with γ -Al₂O₃

$\langle 111 \rangle // \text{Si} \langle 111 \rangle$ in film normal direction and $\gamma\text{-Al}_2\text{O}_3$
 $\langle 1\bar{1}0 \rangle // \text{Si} \langle 1\bar{1}0 \rangle$ in film plane direction.

P6.13

GROWTH OF EPITAXIAL NICKEL OXIDE ON NICKEL BY OXIDATION. Mani Gopal, Michael Cima, Department of MS&E, Massachusetts Institute of Technology, Cambridge, MA.

The increase in molar volume during the oxidation of nickel to nickel oxide is over 65%. This volume change induces a strain in the oxide film, which is accommodated by the nucleation and growth of grains of different orientations. Consequently, NiO grown on Ni is polycrystalline. In this paper, we report on a process of growing epitaxial NiO on single crystal nickel, where the fraction of oriented NiO is over 99%. This high degree of orientation is obtained by controlling the texture of the first few layers of oxide formed on the surface. This layer acts as a template for subsequent growth of thick epitaxial oxide scale. We present the mechanism by which the oxides are formed, and suggest that this approach of growing epitaxial oxides can be extended to other metal and alloys systems.

P6.14

SURFACE MORPHOLOGY AND MICROSTRUCTURE OF COBALT OXIDE FILMS BY LOW TEMPERATURE, LOW PRESSURE MOCVD. Anil U. Mane, Mandar A. Paranjape, Shalini K., and S.A. Shivashankar, K. Chattopadhyay, Materials Research Centre, Indian Institute of Science, Bangalore, INDIA.

Thin film morphology and microstructure are very important because they influence properties relevant to applications such as solar-selective absorption, protective layer coating, and gas sensing. The growth of thin films of oxides by low temperature, low pressure MOCVD often leads to interesting film morphologies and microstructures because growth can occur under far-from-equilibrium conditions. We have studied the growth of thin films of cobalt oxides on a variety of substrates from different metalorganic cobalt complexes, under various growth conditions. For example, it is found that Co_3O_4 films grown from $\text{Co}(\text{II})$ acetylacetonate at low temperatures $\sim 350^\circ\text{C}$ on glass, quartz, and $\text{Si}\{100\}$ consist of crystallites of extremely uniform size and morphology, though oriented at random. This appears to result from a high density of nucleation under a variety of CVD growth conditions. On single crystal substrates, however, highly oriented and epitaxial films grow readily: at substrate temperatures as low as 450°C , the growth of nearly perfect epitaxial films of Co_3O_4 occurs on $\text{SrTiO}_3\{100\}$. Under very similar CVD conditions, growth on $\text{MgO}\{100\}$ leads to epitaxial films of CoO . It is also observed that, besides surface morphology, the chemical composition of the films is affected by the deposition conditions. This is because, without altering the phase of cobalt oxide formed, the carbon content of the film depends on the growth conditions. The inclusion of carbon in the films (which is due to the use of metalorganic complexes as precursor) alters the nucleation and growth processes and, therefore, the microstructure of the films. This affects film properties such as optical absorption. Phase formation, epitaxy, surface morphology, and chemical composition of Co_3O_4 thin films were studied by XRD, SEM, SIMS, and AFM. Optical properties measured by spectrophotometry and ellipsometry will also be reported.

P6.15

FORMATION OF ATOMICALLY FLAT SURFACES ON STRONTIUM TITANATE AND SAPPHIRE. A.P. Li, C. Bednarski, Z. Dai, and B. Golding, Center for Sensor Materials and Department of Physics & Astronomy, Michigan State University, MI.

The SrTiO_3 (100) and $\alpha\text{-Al}_2\text{O}_3$ (0001) surfaces are attractive substrates for the growth of superconductor, metal, semiconductor, and ceramic thin films. Since the quality of thin films is closely related to substrate surface defects, significant effort has been given to the study of the surface treatments required to produce atomically flat surfaces on both substrates. To achieve a high degree of reproducibility, we have developed a well-controlled procedure that results in atomically flat surfaces on SrTiO_3 (100) and $\alpha\text{-Al}_2\text{O}_3$ (0001). Atomic force microscopy has been used to examine the surface structures. As-received SrTiO_3 crystals were carefully cleaned and etched in a buffered NH_4F -HF solution to remove damaged layers. Well-defined and ultra-smooth SrTiO_3 (100) with unit cell height steps of 0.4 nm was obtained by O_2 annealing at 950°C . As-received $\alpha\text{-Al}_2\text{O}_3$ (0001) crystals were chemically cleaned and then etched in a solution of NH_4OH , H_2O_2 and H_2O . With this treatment, facet formation on the surface was observed after annealing in the range of $900\text{-}1200^\circ\text{C}$ in air for short periods. The straight, well-defined terraces have step height 0.2 nm. After 8 hour anneals at 1200°C , we find double steps resulting from the coalescence of single steps of 0.2 nm height. These procedures provide well-defined substrate surfaces for well-regulated epitaxial thin-film growth.

P6.16

ULTRA-THIN ZIRCONIUM SILICATE FILMS WITH GOOD PHYSICAL AND ELECTRICAL PROPERTIES FOR GATE DIELECTRIC APPLICATIONS. Easwar Dharmarajan, Wen-Jie Qi, Renee Nieh, Laegu Kang, Katsunori Onishi and Jack C. Lee, The University of Texas at Austin, Austin, TX.

The need for alternative gate dielectrics to replace conventional SiO_2 is increasing to facilitate further CMOS scaling. Various high-k materials like Ta_2O_5 , TiO_2 , ZrO_2 , HfO_2 have been studied as potential replacements. But some of these materials are not thermodynamically stable in contact with Si and therefore require some barrier layer. One of the most promising materials for use as an alternative gate dielectric is Zr silicate due to its thermodynamic stability on Si and its good interface quality with Si. In this study, ultra-thin Zr silicate films (45-60 angstroms) with different Zr compositions have been deposited on Si using co-magnetron reactive sputtering. The composition variation changes the dielectric constants of these films with the higher Zr composition films having higher k. But, the Zr composition was kept below the stoichiometric composition of 16% to prevent precipitation of ZrO_2 and to have Si rich films for better interface quality. Films were rapidly thermal annealed in N_2 ambient up to 900°C and Pt was used as the gate electrode. Based on the electrical characterization of these films, we demonstrate ultra-thin films with equivalent oxide thickness (EOT) of < 14 angstroms with gate leakage significantly lower than SiO_2 of similar thickness and hysteresis $< 20\text{mV}$. The films also exhibit good thermal stability up to 900°C annealing as shown by a minimal increase in EOT and also remain amorphous at high temperature. Further material analyses include TEM, XPS to characterize the films.

P6.17

A HYDROGEN BONDING BASED NEW APPROACH TO FABRICATE POLYMER/INORGANIC NANOPARTICLES MULTILAYER FILM. Encai Hao and Tianquan Lian, Emory Univ, Dept of Chemistry, Atlanta, GA.

Metallic and semiconductor nanoparticles represent an advanced materials dimension that bridges bulk material and molecular behavior and offers prospects of novel, and even size-dependent, chemical, electronic, and physical properties. The organization of nanoparticles into inorganic-organic heterostructures, mainly by self-assembly method and LB techniques, displays promising characteristics for the preparation of light-emitting diodes, nonlinear optical devices and electrically conductive films. There is great interest in fabricating thin films in the nanometer size range based on new strategies. Recently, hydrogen bonding based approaches to fabricate multilayer polymer films were developed by Rubner et al. using polyaniline[1] and by Zhang et al. using poly(vinylpyridine)/poly(acrylic acid).[2] These studies confirmed that relatively strong secondary forces could be used to assemble multilayer thin films in a layer-by-layer manner. Herein, we report the layer-by-layer assembly of hybrid poly(vinylpyridine)/Inorganic nanoparticles multilayer thin films based on hydrogen bonding. The multilayer buildup was monitored by UV-visible spectra, which showed a linear increase of the film absorbance with the number of adsorbed nanoparticle layers. The resulting films had a high degree of flatness and smoothness as indicated by small angle X-ray diffraction (SAXD). Hydrogen bonding between the pyridine group of poly(vinylpyridine) and the carboxylic acid group on nanoparticles is the driving force for the multilayer film fabrication. This was verified using FTIR spectroscopy.

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P6.18

MODELING THE STRUCTURAL DISJOINING PRESSURE OF THE NEMATIC LIQUID CRYSTAL THIN FILMS. Alejandro D. Rey, McGill University, Dept. of Chemical Engineering, Montreal, Quebec, CANADA.

A mechanical theory of structural disjoining pressure in nematic liquid crystal films is developed based on Laplace's interfacial stress balance equation. Identification of the interfacial stresses in nematic liquid crystal interfaces leads to two contributions to the structural disjoining pressure. It is shown that tensor order parameter gradients across the film give rise to bulk Ericksen stresses, whose normal component results in a disjoining pressure that tends to stabilize the film. In addition, tangential gradients in the tensor order parameter give rise to gradients in interfacial bending stresses whose normal component results in a film pressure that may be disjoining or conjoining. Phenomenological expressions for the two structural disjoining pressures are obtained using the classical equations of liquid crystal bulk and surface elasticity.

P6.19

Abstract Withdrawn.

P6.20

GROWTH FRONT ROUGHENING OF ROOM TEMPERATURE DEPOSITED OLIGOMER THIN FILMS. D. Tsamouras, G. Palasantzas, J.Th.M. De Hosson, and G. Hadziioannou, Department of Polymer Chemistry and Department of Applied Physics, Materials Science Center, University of Groningen, Groningen, THE NETHERLANDS.

Thin films grown under non-equilibrium conditions show in many cases scaling behaviors. Recently there has been an increasing technological interest in organic thin films, either polymers or oligomers, as the active layer in molecular devices such as light-emitting-diodes (LED), solar cells and field-effect-transistors (FET). Therefore, control of the film morphology is of primary concern to anyone working on the optimization of electro-optical properties of organic-based photonic devices. So far, only scant research was concentrated on growth properties of organic thin films showing the possibility of various scaling relations that control their growth morphology. In this work growth front scaling aspects are investigated for PPV-type oligomer thin films vapor-deposited onto silicon substrates at room temperature. For film thickness $d \sim 15$ -300 nm, commonly used in optoelectronic devices, height-difference correlation function measurement by atomic force microscopy yields roughness exponents in the range $H=0.45 \pm 0.04$, and an rms roughness amplitude s which evolves with film thickness as a power law $s \sim d^b$ with $b=0.28 \pm 0.05$. The non-Gaussian height distribution and the measured scaling exponents (H and b) suggest a growth front roughening mechanism close to that described by the Kardar-Parizi-Zhang (KPZ) growth model.

P6.21

Abstract Withdrawn.

P6.22

SELF-ASSEMBLY OF COLLOIDAL PARTICLES ONTO SURFACES OF EMULSION DROPLETS. M.F. Hsu, M. Nikolaidis, A.D. Dinsmore, A.R. Bausch, D.A. Weitz, Harvard Univ, Dept of Physics, Cambridge, MA.

Composite particles with well-controlled elastic and structural properties are of current interest, both for fundamental research and high-technology applications. As shown by others, water droplets in oil can be used as templates upon which latex particles are self-assembled. Latex particles form 2D shells on the templates. However, the fundamental forces involved remain unclear. We will discuss new studies of the interactions between the particles and the oil/water interface. An understanding of these interactions enables us to exert tighter control of physical properties of the resulting latex shells. Measurements of the shell size, elasticity, and latex particle configuration will be presented. Characterization of our samples is done primarily with 3D confocal microscopy. Elastic properties were quantified by measuring the 3D structure and response to macroscopically applied stress. We will conclude with proposals for future work and suggestions for possible applications.

P6.23

GROWTH MECHANISM AND MORPHOLOGY OF FILMS PRODUCED BY VAPOR DEPOSITION POLYMERIZATION. Y.-P. Zhao, J.B. Fortin, G.-C. Wang, and T.-M. Lu, Rensselaer Polytechnic Institute, Dept of Physics, Applied Physics, and Astronomy, Troy, NY.

The roughening mechanisms and morphology of thin films prepared by physical vapor deposition (PVD) processes such as molecular beam epitaxy have been extensively studied in the past. Recently, there are growing technological interests in polymer thin films prepared by vapor deposition polymerization (VDP) for molecular devices and microelectronic interconnects. In a VDP process, the monomer can be consumed by two chemical reactions: initiation, in which new polymer molecules (chains) are generated; and propagation, in which existing polymer molecules are extended to higher molecular weight. The differences between VDP and PVD lie in the nucleation and growth process after the monomers have condensed on the substrate. For the VDP process, the reaction occurs only at the ends of a polymer chain, and surface diffusion, intermolecular interaction, and chain relaxation can occur during growth. These processes are very different from the atomistic processes for PVD, and should give a distinct dynamic behavior of the morphology of VDP film. In the present study, we examine the roughness evolution in the growth of a simple polymer, $-(C_8H_{10})-$, called p-xylylene. The surface morphology has been investigated using atomic force microscopy. The vertical interface width w increases as a power law of film thickness d , $w \sim d^\beta$, with $\beta = 0.25 \pm 0.03$, and the lateral correlation length ξ grows as

$\xi \sim d^{1/z}$, with $1/z = 0.31 \pm 0.02$. This novel scaling behavior is interpreted as the result of monomer bulk diffusion, and belongs to a new universality class that has not been discussed previously. Work supported in part by NSF.

P6.24

MOLECULAR ORIENTATION IN THE PEPTIDE SELF-ASSEMBLED MONOLAYERS. Katsuhiko Fujita, Ryuichi Yokoyama, Tetsuo Tsutsui, Kyushu Univ, Dept of Appl. Sci. for Electronics and Materials, Fukuoka, JAPAN.

Thiol or disulfide derivatives spontaneously form self-assembled monolayers (SAMs) on gold and silver substrates by the immersion of the substrates into the solutions. The closely packed organic films have been investigated to vary the properties of metal/organic contact. Helical peptides carrying a large dipole moment along the helix axis are considerable candidates to control the electric property at the interface. Two kinds of helical peptides, Peptide I and II were synthesized to fabricate peptide SAMs. Peptide I has a disulfide group at an N terminal and Peptide II at a C-terminal. Each peptide can bind on a gold substrate at the disulfide moiety, resulting the opposite direction of the dipole in the SAM. The thickness of the SAMs was determined with surface plasmon resonance and X-ray reflectivity and the molecular orientation angle from the surface normal was estimated with IR-RAS. The work functions of the gold covered with the SAMs are estimated using ultraviolet photoelectron spectroscopy. The thickness of the monocomponent SAMs roughly agreed with the helix diameter. On the other hand, that of the equimolar mixed SAM corresponded to the molecular length along the helix axis. The ratio of amide I band and amide II band in IR-RAS revealed that the monocomponent SAMs have much larger tilt angle from the surface normal than the equimolar mixed SAM. These observations indicate that the helical peptides were closely packed and vertically oriented in the equimolar mixed SAM though they lying flat on the interface in the monocomponent SAMs. The molecular orientation will be discussed in terms of the interaction of the aligned dipole and the substrate. This work is partly supported by Core Research for Evolutional Science and Technology of Japan Science and Technology Corporation (CREST/JST)

P6.25

FABRICATION OF MULTILAYER FILMS USING A SPINNING PROCESS. Jinhan Cho, Kookheon Char, Seoul National University, School of Chemical Engineering, Seoul, KOREA; Jong-Dal Hong, University of Inchon, Department of Chemistry, Inchon, KOREA; Ki-Bong Lee, Pohang University of Science and Technology, Department of Physics, Pohang, KOREA.

We introduce a new method to build up ultrathin multilayer films composed of cationic poly(allylamine hydrochloride) (PAH) and anionic poly(sodium 4-styrenesulfonate) (PSS) using a spinning process. Since the deposition of each polymer layer is carried out at a high rotation speed, the adsorption time for the formation of a homogeneous thin layer requires only 15 seconds. The adsorption process of the spin-assisted self-assembly method applied to present work is mainly driven by both the viscous force by fast solvent elimination and the electrostatic interactions between oppositely charged species. On the other hand, the centrifugal and air shear forces caused by the spinning process significantly increase the desorption of weakly adsorbed polyelectrolyte chains and the planarization of the adsorbed polyelectrolyte layer. By the combination of the four different forces mentioned above, the adsorbed film thickness per bilayer could be easily controlled from about 0.5 nm to 4 nm by varying the rotation speed and mole concentration of polyelectrolytes. It is also demonstrated that the surface of the multilayer films is quite homogeneous and smooth, indicating a surface roughness below 0.5 nm, as evidenced from X-ray reflectivity and atomic force spectroscopy (AFM).

P6.26

ADSORPTION AND ORDERING OF CHARGED COLLOIDS ON INHOMOGENEOUSLY CHARGED SURFACES. Babak Sadigh, Michael P. Surh, William D. Wilson, Lawrence Livermore National Laboratory, Livermore, CA.

We have developed a grand-canonical Brownian dynamics (G CBD) simulation scheme to study the adsorption of the spherical colloid particles on surfaces, interacting through DLVO potential plus short-range hydrophobic attraction forces. The surface is represented as a charged sheet attracting the colloid particles through a screened Coulomb potential. Our formalism allows for an inhomogeneous charge distribution on this surface. In particular we perform extensive simulations to study the effect of layered surfaces - e.g. laminates - on the ordering of the adsorbed particles. This scheme can be readily extended to the simulation of more complicated cases such as non-spherical or composite particles. It is also relevant to protein crystal growth. This work was carried out under the auspices of the

P6.27

NUCLEATION AND GROWTH OF COLLOIDAL HARD SPHERE CRYSTALS. Urs Gasser, Eric R. Weeks, David A. Weitz, Harvard University, Division of Engineering and Applied Sciences, Cambridge, MA.

We use suspensions of colloidal particles to study the nucleation and growth of colloidal crystals. Our particles have a diameter of about 2 microns, are dyed with rhodamine and sterically stabilized. They closely approximate hard spheres. As solvent we use a mixture of decalin and cyclo-hexyl bromide, which allows to both index- and density-match the PMMA particles.

The evolution from the unordered metastable liquid to the crystalline phase is observed with a laser scanning confocal microscope which makes it possible to determine and follow the positions of roughly 5000 particles in the sample while it crystallizes. This makes it possible to study a single crystalline nucleus as it reaches the critical size and its evolution to a large crystal grain. We use local bond order parameters to identify crystal like particles or regions. By analyzing and tracking the crystalline clusters that form during a measurement we are able to extract information about the free energy barrier such as the surface energy and the morphology of the crystallites.

P6.28

SELF-ASSEMBLY OF RUTHENIUM PORPHYRINS INTO MONOLAYER AND MULTILAYER ARCHITECTURES VIA HETEROGENEOUS COORDINATION CHEMISTRY. David M. Sarno, Wayne E. Jones, Jr., State University of New York at Binghamton, Department of Chemistry and Institute for Materials Research, Binghamton, NY; Luis J. Matienzo, IBM Corp., Endicott, NY.

A fuller understanding of the relationships between physical structure and properties is the key to the development of new materials for use in light emitting diodes (LEDs), chemosensors, and light-harvesting devices. These technologies have utilized porphyrins and other chromophores as polymers and spin-coated thin films on a variety of substrates. Unfortunately, it is difficult to separate inter- and intramolecular interactions in amorphous films. Building on our successful preparation of polymer multilayer structures, we have developed a self-assembled molecular architecture composed of Ruthenium (II) tetraphenyl porphyrin (carbonyl) molecular units anchored to a monolayer of pyridine-terminated alkylsilanes on silica substrates. Following exposure of the pyridine-terminated surface to the porphyrin, UV-vis spectroscopy reveals the porphyrin Soret absorption at 412 nm, which persists even after vigorous washing. Further evidence of coordination is obtained from XPS analysis, which reveals a slightly broadened N 1s signal shifted to a higher binding energy of 399.7 eV, relative to the energies of unbound porphyrin (399.1 eV) and pyridine (399.3 eV). The strongly bound carbonyl ligands on the chromophores inhibit the formation of multiple amorphous layers under ambient conditions. However, a multilayer system can be prepared via photodecarbonylation in the presence of dipyriddy spacers in solution, allowing coordination of additional porphyrin units. More highly organized systems are now being explored which utilize tetrapyriddy metalloporphyrins capable of coordination into larger planar arrays for subsequent incorporation into extended multilayer architectures. The morphology of these thin films can be examined by AFM in order to confirm formation of regular multilayer structures.

P6.29

STEARIC ACID MONOLAYER GROWTH AT STEPPED SAPPHIRE SURFACES. Chad Taylor and Dan Schwartz, Tulane University, Dept of Chemistry, New Orleans, LA.

Stearic acid monolayer growth at annealed sapphire substrates of crystal orientation (0001) and (1102) (C- and R-plane Al_2O_3 , respectively) has been monitored by in-situ and ex-situ atomic force microscopy (AFM), contact angle measurements, and transmission infrared spectroscopy (IR). When annealed at 1300°C, these bare surfaces are microscopically smooth with uniform terrace widths and step heights, the dimensions of which prove to be dependent on the crystal orientation and the angle of miscut from the nominal plane. Importantly, the termination layer consists of Al atoms for the C-plane surface and O atoms for the R-plane surface. AFM images indicate the stearic acid molecules are indifferent to the adsorption site – step edge or terrace. Thus, monolayer growth kinetics discerned from our characterization techniques are rationalized on the basis of these differences in crystal orientation surface chemistry.

P6.30

MOLECULAR MECHANISM IN THE ORDERED GROWTH OF LAYER-BY-LAYER ASSEMBLED ZINC-BISQUINOLINE FILMS.

F. Papadimitrakopoulos, J. Mwaure, K. Ray, T. Phely-Bobin, R. Tipnis, Dept of Chemistry, Polymer Science Program, Nanomaterials Optoelectronic Laboratory, Institute of Materials Science, University of Connecticut, Storrs, CT.

The layer-by-layer deposition of conformal thin films from a variety of organic or inorganic materials have proved to be a powerful technique in constructing multi-component molecular architectures with precisely controlled thicknesses. Our group has previously reported on the metalorganic assembly of thin films using 8,8'-dihydroxy 5,5'-bisquinoline (bisquinoline) and diethyl zinc (as the zinc precursor). In this paper, we have utilized different zinc precursors (ZnEt_2 , ZnCl_2 , ZnBr_2 , $\text{Zn}(\text{CH}_3\text{COO})_2$, and $\text{Zn}(\text{CF}_3\text{COO})_2$) in the assembly of zinc-bisquinoline films. These assemblies were characterized through a series of analytical tools to obtain a more comprehensive picture of their underlying structure and explain the molecular mechanism involved in their growth. Utilizing carefully engineered substrates, we demonstrated a novel phenomenon associated with the zinc-precursor, and in particular a certain fraction of it, which is labile. The accelerated growth observed is presently explained via a secondary self-assembly process of labile zinc-precursors stabilized within cavities formed in the primary structure. Increasing the order within these assemblies was shown to decrease their photoluminescence efficiency.

P6.31

UNIQUE FEATURES OF THE CRYSTALLIZATION KINETICS OF FeCrBSi THIN FILMS OBTAINED BY LASER ABLATION DEPOSITION. M. Sorescu, A. Grabias, Duquesne University, Department of Physics, Pittsburgh, PA.

Pulsed laser deposition was used to obtain a metallic glass in a thin film form using the amorphous $\text{Fe}_{77}\text{Cr}_2\text{B}_{16}\text{Si}_5$ ribbon as a target. Glass substrates were used. The as-deposited films were annealed in the same conditions as the ribbon samples in order to compare their crystallization behaviors. Transmission Mössbauer measurements were performed to determine the crystallization products formed due to annealing of the $\text{Fe}_{77}\text{Cr}_2\text{B}_{16}\text{Si}_5$ ribbon. Conversion electron Mössbauer spectroscopy (CEMS) was used to obtain structural and magnetic information from the thin films as well as from the surface layers of the ribbons about 100 nm thick. All measurements were done at room temperature as a function of annealing temperature (up to 600°C). The transmission Mössbauer spectra revealed the formation of both the bcc-FeSi and bct- $\text{Fe}_3(\text{Si}_2\text{B})$ phases in the bulk of the annealed ribbons. However, at the surfaces of the ribbons annealed at higher temperatures, the bcc-Fe, bcc-Fe(Si) and tetragonal Fe_2B phases were detected. These results are clearly different from those obtained for the metallic glass thin films. Indeed, the CEMS spectrum recorded for the as-deposited film shows that the film is fully amorphous. After annealing at 450°C the film crystallized completely, consisting of a complex mixture of phases observed for the crystalline ribbons and iron oxides. However, the thin film annealed at 550°C reveals only one iron-containing phase with hyperfine field of 51.8 T. The hyperfine parameters indicate that this phase could be Fe_2O_3 . Our Mössbauer study showed that the crystallization kinetics of the thin films of FeCrBSi is different from the crystallization mechanism of the bulk ribbon.

P6.32

LOW-FIELD MAGNETORESISTANCE PROPERTY OF $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$ THIN FILMS WITH NANO-CRYSTALS EMBEDDED IN AMORPHOUS MATRIX. J.-M. Liu, Z.-G. Liu, Nanjing University, Laboratory of Solid State Microstructures, Nanjing, CHINA.

$\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$ (LSMO) thin films on quartz wafers at different deposition temperatures have been prepared using pulsed laser deposition. The microstructural, electrical and low-field magnetotransport properties of these films are evaluated as functions of the deposition temperature. The film crystallinity depends largely on the deposition temperature. Significantly enhanced low-field magnetoresistance for the samples deposited from 570°C to 600°C in which nano-crystals are embedded in the amorphous matrix. The electrical and low-field magnetotransport property of the thin films is well explained in terms of the two-channel model where the insulating channel of variable range hopping conduction and metallic one coexist in parallel.

P6.33

CRYSTALLIZATION OF LANTHANUM STRONTIUM COBALT OXIDE THIN FILMS FROM AMORPHOUS PRECURSORS. Hauyee Chang, Yi Dong, Lawrence Berkeley National Laboratory, Berkeley, CA; Songye Chen, Chonglin Chen, Paul CW Chu, Dept. of Physics, University of Houston, Houston, TX.

It is well-known that $(\text{La,Sr})\text{CoO}_3$ (LSCO) is a good conductor. Therefore, it is very commonly used as bottom electrodes for various

devices. It is interesting to note that amorphous LSCO thin films are actually non-conducting and translucent. On annealing at temperatures above 600°C, the amorphous thin film becomes metallic and looks shiny and opaque. However, there have been very few studies done on this interesting process. We have made amorphous LSCO thin films by depositing the films onto room temperature substrates (LaAlO₃). The electrical resistances of these films are monitored as they are heated to high temperatures. Two distinct phase transitions are observed with abrupt changes in the electrical resistance of the films. These changes are most likely associated with transitions from non-ohmic to ohmic and semi-conducting to metallic. X-ray diffraction studies show that the annealed films are (001) oriented on (001) LaAlO₃ (LAO) and they tend to grow in a cube-on-cube fashion on LAO.

P6.34

β -FeSi₂ THIN-FILMS GROWN BY A PULSED LASER DEPOSITION METHOD. S. Uekusa, Y. Watanabe, N. Miura, Y. Aida, Meiji Univ, Kawasaki, JAPAN.

Orthorhombic β -FeSi₂ behaves as semiconductor with a direct band gap of about 0.85 eV, and shows a large Seebeck coefficient and optical absorption coefficient ($>10^5$ cm⁻¹ at photon energies above 1.0 eV). Furthermore, it is composed of nontoxic elements, which exist in great abundance on earth. Therefore, the use of β -FeSi₂ is expected in applications of thermoelectric devices, light emitting devices and photovoltaic cells. In this study, we attempted to grow β -FeSi₂ thin-films on Si substrate, using a pulsed laser deposition method. Both n-Si(100) and n-Si(111) single crystal were used as the substrates because β -FeSi₂ was found to be a p-type semiconductor. The substrates were first cleaned with organic solvents. After being rinsed in high purity water, they were dipped in a dilute HF solution in order to remove the native oxide. Subsequently, the substrate was loaded into growth chamber with the base pressure below 10⁻⁵ Pa. β -FeSi₂ thin-films were grown by various substrate temperatures. In order to determine the phase of silicide layer and measure the band gap energy value, X-ray diffraction (XRD) measurement and transmittance measurement were carried out, respectively. From the results of the XRD measurement, when the substrate temperature was 500°C, β -FeSi₂ thin-films grew both Si(100) and Si(111) substrate. We made it clear that β -FeSi₂ thin-films grown on Si(100) substrate were a polycrystalline structure, but thin-films grown on Si(111) substrate were a monocrystalline structure. The value of band-gap energy calculated from the results of transmittance measurement was about 0.75 eV. This value is smaller than it reported previously. We consider that the reason is due to Si-rich composition in β -FeSi₂ thin-films. We report that relationship between band-gap energy and composition in β -FeSi₂ thin-films on Si substrate.

P6.35

THE EFFECT OF SURFACE TOPOGRAPHY ON GRAIN GROWTH IN Al FILMS. C.A. Volkert and S. Bähr, Max-Planck-Institut für Metallforschung, Stuttgart, GERMANY.

The effect of surface topography on grain growth and texture evolution in Al thin films on Si substrates has been investigated. The film surface was planarized by compressing it during annealing with either flat or patterned punches. Following annealing, the microstructure in the compressed and uncompressed regions was compared using FIB microscopy, AFM, EBSD, and x-ray diffraction. It was observed that the grains in the compressed regions were up to 4 times larger than in the uncompressed regions and had a stronger (111) texture. By performing tests under different applied compressive stresses it was concluded that the enhanced grain growth is not driven by either the stresses or plastic strain energy, but rather by the removal of the grain boundary grooves at the surface, which act as pinning sites for grain boundary motion. This picture is supported by the fact that compression with punches with appropriate surface topography could be used to replicate the surface pattern in the grain structure of the film. Due to the fact that the Si substrates were not completely flat, homogeneous compression of the film surface was not possible and tests are now being performed on Al films deposited on compliant Kapton substrates, with the hope of obtaining more systematic results.

P6.36

GROWTH OF THIN FILMS OF SUPERIONIC PbSnF₄: INFLUENCE OF THE REACTION MEDIUM AND PHASE TRANSITIONS, AND RESULTING ANISOTROPIC PROPERTIES. Georges Dénès and M. Cecilia Madamba, Concordia University, Dept. of Chemistry and Biochemistry, Laboratory of Solid State Chemistry and Mössbauer Spectroscopy, and Laboratories for Inorganic Materials, Montréal, Québec, CANADA.

PbSnF₄ is the highest-performance fluoride ion conductor known to date, i.e. three orders of magnitude higher than β -PbF₂, which is the best for fluorides containing only one kind of metal ions. Its

exceptionally high fluoride ion conductivity has been applied to the fabrication of a chemical sensor. We showed in earlier works that there are many ways to prepare PbSnF₄, and depending on the method of preparation and subsequent treatments, a large number of different polymorphs are obtained. In addition, several phase transitions, mostly of the order-disorder type, are observed, making this material one of the most complex known, despite the deceiving simplicity of its chemical formula. The crystal structure of all phases of PbSnF₄ is related to that of fluorite-type β -PbF₂, either with full or partial ordering between Sn and Pb, which results in superstructures and lattice distortions, with highly anisotropic properties, or with full disorder, resulting in cubic unit-cells and no superstructure. In ordered phases, the tin(II) non-bonded electron pair (lone pair), which is stereoactive in all cases, cluster in planes. No bonding can occur through the planes of lone pairs, which are therefore very efficient cleavage planes. This results in assemblies of very thin sheets (nanothick) parallel to one another, giving a very highly lamellar structure. The present work was focussed on the enhancement of the thin film alignment, and its evolution through the α - to α -PbSnF₄ phase transition, where the ferroic nature of the transition reduces the alignment. The implications on the anisotropy of the properties will also be examined.

P6.37

KINETICS OF NITROGEN INCORPORATION IN THERMAL SILICON DIOXIDE BY RADIO-FREQUENCY PLASMA ASSISTED ELECTRON CYCLOTRON RESONANCE. Jason Brewer, Avi Raveh, Eugene A. Irene, University of North Carolina at Chapel Hill, Dept of Chemistry, Chapel Hill, NC.

The kinetics of nitrogen incorporation and silicon nitride (Si₃N₄) formation in conventional thermal silicon dioxide (SiO₂) films by dual-frequency plasma were studied. The nitridation of the SiO₂ films was performed in nitrogen plasma sustained by radio-frequency discharge and/or electron cyclotron resonance. The effect of the nitridation time, substrate temperature, and gas pressure on the nitrogen content and on the Si₃N₄ volume fraction in the oxide films were examined by means of Auger electron spectroscopy (AES), Fourier transform infrared (FTIR) spectroscopy, and spectroscopic ellipsometry (SE). It was observed that the formation of the Si₃N₄ ceased after 30 min of nitridation. This time was found to decrease when higher RF voltage was applied in combination with the ECR. At longer times, the enhancement of nitrogen diffusion into the bulk oxide layer is governed by the electric field and by the high nitrogen concentration gradient on the nitrided surface. FTIR analysis indicated that the nitrided films were composed of Si₃N₄, SiO₂, and SiO. AES analysis revealed that the N/(Si O N) ratio in the nitrided layer was higher for films nitrided by ECR/RF plasma when compared with those nitrided by RF plasma alone. In addition, thermal stability studies indicated that the highest bonded nitrogen content was obtained with the ECR/RF plasma.

P6.38

SURFACE EVOLUTION OF NiTi AND NiTiHf THIN FILMS. Chen Zhang, Ralph H. Zee, Auburn University, Materials Research and Education Center, Auburn, AL; Paul E. Thoma, Johnson Controls, Inc., Corporate Technology, Milwaukee, WI.

The microstructure evolution of Ti-rich NiTi thin films and (TiHf)-rich NiTiHf thin films containing 9at% Hf was investigated. These films were deposited from single NiTi and NiTiHf targets using a DC magnetron sputtering system. Free-standing films were obtained by using single crystal silicon substrates. The thickness of these films was controlled between 10-12 μ m. In this investigation, the effects of deposition temperature on the surface and cross-sectional microstructures of these films were studied. Substrate temperature during deposition was varied between 300°C to 700°C at 100°C intervals. The influence of post deposition heat treatment temperature on the microstructure of these films was also studied. The post deposition heat treatment temperature was varied between 300°C and 800°C at 100°C intervals. Both surface and cross-sectional microstructures were examined using a scanning electron microscope (SEM). Transformation temperatures of these films were determined by differential scanning calorimetry (DSC), and the crystallinity was determined using x-ray diffractometry. All the as-deposited films were found to be crystalline, even when the substrate temperature was as low as 300°C. Results from the microstructure analysis show that all the films have a relatively fine grain size ranging from 0.2 μ m to 2.5 μ m, and the grain size increases with increasing substrate deposition temperature. The effect of post deposition heat treatment on grain size was found to be minimal.

P6.39

Abstract Withdrawn.

P6.40

OPEN-SHELL TIGHT-BINDING MOLECULAR DYNAMICS

SIMULATION STUDY ON THE CHEMICAL VAPOR DEPOSITION PROCESSES. Seichi Takami, Hitoshi Kurokawa, Ken Suzuki, Momoi Kubo, Akira Miyamoto, Tohoku Univ, Dept of Materials Chemistry, Sendai, JAPAN; Akira Imamura, Hiroshima Kokusai Gakuin Univ, Dept of Mathematics, Hiroshima, JAPAN.

The development of silicon technology reduced the size of device structures, requiring the control of preparation processes of the devices at an atomic level. This trend increased the importance of molecular simulation of the elementary processes of device preparation method including chemical vapor deposition processes. Such elementary processes involve the dynamic displacement as well as the change in the electronic state of the atoms. Therefore, computational methods have to consider and reproduce the dynamics of both the atomic and electronic state. We have developed an open-shell tight-binding molecular simulation code that enabled us to study the dynamics of a molecular system while considering the electric state with a considerable reduced computational load. In addition, this program can handle spin-up and spin-down electrons, facilitating the study of chemical reactions that involve radical reactions. This presentation focuses the application of the program to study chemical reactions such as deposition of SiH_3 radicals on a Si(100) surface.

P6.41
MONTE CARLO SIMULATION OF CVD DEPOSITION OF NONSTOICHIOMETRIC AMORPHOUS SILICA. V.M. Burlakov, A.P. Sutton, G.A.D. Briggs, Department of Materials, University of Oxford, Oxford, UNITED KINGDOM; Y. Tsukahara, Technical Research Institute, Toppan Printing Co Ltd., Saitama, JAPAN.

The model suitable for simulation of CVD growth of amorphous Si and SiO_x is proposed. It is based on the network properties of the materials and essentially involves dangling bonds arising during the real process of deposition. Interatomic interaction is described within Keating-like valence force model (*P.N. Keating, Phys. Rev. 145, 637 (1966)*) with additional repulsive force between nonbonded atoms. Single bond formation/breaking and dangling bond diffusion are considered as elementary steps for sampling the system phase space in the Metropolis MC scheme. Simulated structures are characterized by radial- and bond angle distribution functions (RDF and BADF, respectively), SiO rings statistics and porosity. RDFs calculated for the simulated amorphous silicon and silica agree well with those obtained experimentally for the bulk materials. The final structures are found to be porous with different mechanisms of pore formation in boundary compounds (Si and SiO_x). Porosity in amorphous Si is quite low (< 3%) almost regardless the nucleation sites density (NSD) on the substrate surface and is associated with structural defects (local breaking of chemical bonds). Silica layers can have much higher porosity (up to 20%) which is strongly dependent on NSD and does not involve any defect formation. Transition from one to the other dominant mechanism of pore formation gradually occurs upon increase of x from 0 to 2.

P6.42
Abstract Withdrawn.

P6.43
LOW TEMPERATURE TUNGSTEN FILM GROWTH AND POST-GROWTH CARBIDATION. Yanfming Sun, Song Yong Lee, Nicholas Nguyen, John G. Ekerdt, John M. White, The University of Texas, Texas Materials Institute, Austin, TX; Ismail Emesh, Motorola, Advanced Products Research and Development Laboratory, Austin, TX.

Low temperature chemical vapor deposition of tungsten films on $\text{SiO}_2/\text{Si}(100)$ surfaces and post-growth treatment with ethylene and ammonia were studied by X-ray photoelectron spectroscopy (XPS) and electron microscopy. Tungsten films were deposited from the $\text{W}(\text{CO})_6$ precursor over temperatures ranging from 250 to 500°C. These films contained approximately 13% C and 6% oxygen as determined by XPS. The growth temperatures were consistent with pyrolysis studies that indicated $\text{W}(\text{CO})_6$ decomposition within a temperature range of 150°C to 200°C. Cross section scanning electron microscopy imaging of the films grown at various temperatures show polycrystalline microstructure, and the grain size increases dramatically as the growth temperature increases. The carbon and oxygen chemical states indicate carbide and oxide formation. Post-growth treatment with ethylene and ammonia at temperatures ranging from 275 to 500°C show carbon and nitrogen content increased, with a significant carbon increase at 500°C. Both graphitic and carbidic carbon were incorporated. The tungsten films also were treated with methane and nitrogen plasma for comparison. Finally, films with and without post-growth treatment were tested as a copper diffusion barrier.

P6.44
INVESTIGATION OF GaN EPILAYERS GROWTH MECHANISMS

USING IN-SITU REFLECTANCE IN MOCVD. O. Briot, M. Moret, S. Ruffenach-Clur, R.L. Aulombard GES, Univ Montpellier II, Montpellier, FRANCE.

GaN is a wide gap semiconductor which is now used to produce blue and green light emitting diodes, blue laser diodes and which has numerous other potential applications, like high frequency HEMT transistors, UV sensors, etc. A complicated two steps process, using a low temperature buffer layer, subsequently annealed and followed by the deposition of the monocrystalline semiconductor was developed, and due to the excellent results obtained following this method, a rush towards applications resulted. There is now a need to investigate in more details the growth mechanisms, and the influence of the growth parameters, in order to ensure a better reproducibility of the results. In this paper, we report an investigation of the growth mechanisms and the influence of the growth parameters using in-situ reflectance experiments. The reflectance measurements allow us to follow the growth rates, and the changes in the surface morphology (transitions between islands growth and 2D growth). Additional ex-situ measurements (AFM and MEB) were performed at different stages of the growth process to ensure additional information. As a result, we demonstrate that the recrystallization of the low temperature buffer layer is a critical step, which is drastically influenced by the composition of the annealing atmosphere (amount of ammonia present in the gas phase), while the deposition temperature and buffer thickness have a moderate effect. We will discuss here the growth mechanisms which may be involved to explain such a behavior.

P6.45
ATOMISTIC SIMULATION STUDIES OF PLASMA-ENHANCED CHEMICAL VAPOR DEPOSITION OF HYDROGENATED AMORPHOUS SILICON FILMS. Shyam Ramalingam, Saravanapriyan Sriraman, Eray S. Aydil, and Dimitrios Maroudas, Dept. of Chemical Engineering, University of California, Santa Barbara, CA.

A systematic computational analysis is presented of the deposition of hydrogenated amorphous silicon (a-Si:H) films on crystalline silicon substrates with H-terminated Si(001) surfaces from silane containing plasmas. Special emphasis is placed on the identification of the elementary surface chemical reactions that govern the deposition process, the amorphous network growth mechanism, and the structural and compositional characterization of the deposited film. The deposition process is modeled by molecular-dynamics (MD) simulation of repeated radical impingement on the growth surface. More importantly, the MD simulations are used to identify elementary surface reactions. The corresponding reaction energy landscapes are computed along the reaction paths based on molecular-statics calculations and the energy levels of reactant, transition-state, and product configurations are computed accurately based on density-functional theory. Our MD simulations reveal a broad class of surface reactions that play important roles in the amorphous film deposition process. Silicon incorporation into the growing film occurs through insertion reactions into Si-Si surface bonds, as well as radical attachment to surface dangling bonds. Surface hydrogen can be removed by abstraction according to Eley-Rideal mechanisms or through a Langmuir-Hinshelwood mechanism that involves formation and desorption of surface silane species. In addition, reactions that involve Si-Si bond formation between adsorbed species are identified and analyzed, as well as various surface migration mechanisms for mobile surface species, such as silicon trihydrides and surface disilane species. The evolution of the film's structure, surface morphology and roughness, surface reactivity, and surface composition also is analyzed systematically. Finally, our simulation results are compared with experimental data from ATR-FTIR spectroscopy. The computed temperature dependence of the H coverage of the surface is in excellent agreement with the experimental data. The predicted surface hydride content also is in good agreement with the experimental measurements. The comparisons are used to discuss our current understanding of the deposition mechanism.

P6.46
MECHANISMS IN EMBEDDED SELECTIVE AREA EPITAXY AND OVERGROWTH OF AN INTEGRATED LASER/MODULATOR QUANTUM WELL STRUCTURE USING MOVPE AND MOVPE. Philipp Kröner^{1,2}, H. Baumeister¹, R. Gessner¹, J. Rieger¹, M. Schier¹, E. Veuhoff¹, O. Marti², H. Heinecke. ¹Infinitec Technologies, Corporate Research CPR PH, Munich, GERMANY; ²University of Ulm, Dept. of Experimental Physics, Ulm, GERMANY.

Laterally integrated laser/modulator structures for 1.55 μm wavelength form a desirable package for long haul high speed optical data transmission. A three-step epitaxial process involving the separate growth of the laser and the modulator structure, finally overgrown with a common cladding, allows for independent process optimization. Here the MOVPE growth of the GaInAsP multiple quantum well (MQW) laser structure on a (001) InP substrate is

applied, a SiN_x stripe mask is deposited and 400 nm deep trenches are etched into the mask openings by reactive ion etching. Following a wet chemical etch step controlling the mask undercut, a MQW electroabsorption modulator structure is selectively filled into the trenches by MOMBE. As major focus we will present the role of the trench wall profile, surface restructuring induced by surface mass transport during pre-growth thermal cleaning and the influence of growth rates and V/III ratios for quantum wells and all other layers. Optimizing those parameters allows for a planar butt coupling to the laser structure. Growth nonuniformities can be limited to a stripe of 500 nm width adjacent to the mask edge. Thus, optical coupling losses from the laser to the modulator structure will be much smaller than in comparable structures grown by MOVPE where the non-uniformities extend for several tens of micrometers. After removal of the mask, a common p-doped InP cladding and a GaInAs contact layer are grown over the integrated structure by MOVPE. TEM analyses reveal a severe dislocation generation in the cladding above the laser/modulator coupling caused by a large local lattice mismatch. Consequently, reactive ion etching is the way of choice for the subsequent ridge waveguide fabrication instead of dislocation sensitive standard wet chemical etching. This overall optimized process sequence is mandatory for the device preparation.

P6.47

A STUDY OF NUCLEATION AND GROWTH IN MOCVD: THE GROWTH OF THIN FILMS OF ALUMINA. M.P. Singh, S. Mukhopadhyay, and S.A. Shivashankar, K. Chattopadhyay, Materials Research Centre, Indian Institute of Science, Bangalore, INDIA.

Though metalorganic chemical vapor deposition (MOCVD) processes have been developed for the preparation of thin films of a wide variety of materials, nucleation and growth in such processes have not been studied in much detail, in part because of the complexity of the chemical processes involved. We have attempted to study these aspects of the MOCVD process using the growth of alumina thin films as an illustration, because thin films of alumina are important as cutting tool material and, prospectively, as the gate oxide in MOSFET devices. Deposition of alumina films was carried out on various substrates such as Si{100} and cemented carbide, in a horizontal, hot-wall, low pressure reactor built in house. Several aluminum β -diketonate complexes were used as the CVD precursor. We have studied nucleation and growth process as a function of different CVD parameters such as total reactor pressure, flow rates of gases, and substrate temperature during film growth. Films have been characterized using optical microscopy, XRD, SEM, and cross-sectional SEM. The chemical composition of the films and of the film-substrate interfaces was determined by Auger depth profiling. Carbon present in the film directly affects the optical properties of thin films, which we have investigated by using spectrophotometry. The nature of the nucleation and growth process was also studied by Monte Carlo simulation. The simulated pattern and experimental process have been compared. Simulation have been carried out based on the lattice-gas model wherein atoms having unit volume occupy a unit cell of the same volume on the substrate, and considering the substrate as a square lattice. For performing the simulation, we have assumed that organic byproducts of the deposition process are volatile and desorb from the substrate surface immediately after dissociation, and that dissociation takes place in a single step.

P6.48

AFM AND TEM EXAMINATION OF SURFACE GRAINS IN LPCVD SILICON FILMS. Dave (Boris) Kharas, R.J. Gambino, State University of New York at Stony Brook, Dept. of Materials Science, Stony Brook, NY; N. Golubovic, Standard MEMS Inc., Hauppauge, NY.

Polycrystalline silicon is an important technological material in microelectronics and more recently in microelectromechanical systems (MEMS). For MEMS applications polysilicon films with residual tensile stress are often used, requiring film growth in the transition zone from 550-600°C. In this study polysilicon films were grown in a hot-walled LPCVD reactor at 590°C to a thickness of 450 nm on p-type silicon substrates. The tensile as-deposited stress in the films was found to decrease with distance from the reactor front and served as a marker for the films changing microstructure and surface roughness as measured by Transmission Electron Microscopy (TEM) and Atomic Force Microscopy (AFM). It was found that the surface contained a high density ($\approx 30/\mu\text{m}^2$) of grains that protruded 30 nm above the mean film surface. The density and volume of these grains increased linearly with decreasing stress until the surface saturated and became uniformly rough. The nature of these surface grains, their spatial characteristics and their annealing behavior is discussed.

P6.49

MODELING MOCVD GROWTH OF YBCO THIN FILMS. Tak Shing Lo, Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University, New York, NY.

YBCO thin film growth by metallorganic chemical vapor deposition (MOCVD) is a complex process involving multiple chemical species. It is therefore natural to seek a model with the capacity to couple growth with surface chemistry, i.e. one that discusses the surface adatom densities of different compounds on the film explicitly. Most traditional growth models do not have this property. A model of this kind, which is a continuum limit of a Monte-Carlo model capturing a caricature of the physics on the atomic length scale has been developed by Schulze and E recently. Here we carry out a numerical study of a phenomenological growth model with terms similar to that of Schulze and E, by coupling it to a 1-D low Mach number flow model for a MOCVD reactor. We include evaporation of surface adatoms, which is the mechanism by which the growth model influences the flow; and a phenomenological nucleation term specifically designed to capture spiral-mode growth in our simulations. We have estimated the parameters of the model by comparing computed solutions to experiments, and examined the consequences of changing various parameters such as the evaporation time. Films that are initially rough are observed to coarsen with time.

P6.50

X-RAY SCATTERING STUDY OF CHEMICAL VAPOR DEPOSITION OF PbTiO₃ THIN FILMS. M.V. Ramana Murty, G.B. Stephenson, S.K. Streiffer, J.A. Eastman, O. Auciello, G.-R. Bai, Materials Science Division, Argonne National Laboratory, Argonne, IL; C. Thompson, Department of Physics, Northern Illinois University, DeKalb, IL and Materials Science Division, Argonne National Laboratory; and A. Munkholm, Chemistry Division, Argonne National Laboratory, Argonne, IL.

Thin films of Pb(Zr_xTi_{1-x})O₃ and related perovskite materials have attracted much attention for integration into a variety of microelectronic applications, including nonvolatile memories, pyroelectric imaging devices, and microelectromechanical actuators/transducers. Metal-organic chemical vapor deposition (MOCVD) can be used to deposit high-quality epitaxial films of oxides with controlled stoichiometry. However, the high pressure and reactive environment of MOCVD has limited fundamental studies of the growth process due to the lack of surface sensitive probes. As a model system, we have investigated PbTiO₃ homoepitaxy and heteroepitaxy on SrTiO₃(001) substrates using *in situ*, real-time x-ray scattering at the Advanced Photon Source. Tetraethyl lead (TEL), titanium isopropoxide (TIP), and O₂ were used as the precursors. We find that PbTiO₃ grows in a layer-by-layer fashion on SrTiO₃ at 650 - 750°C. The films grow coherently (with in-plane lattice parameters matched to the substrate), resulting in a tetragonal distortion of the unit cell. Homoepitaxy of PbTiO₃ was investigated as a function of temperature, growth rate, and the ratio of the precursor (TIP/TEL) flow rate. For the range of TIP/TEL ratios investigated, the film growth rate was found to be proportional to the TIP flow rate. The dependence of PbTiO₃ film structure and morphology on the growth process will be discussed as determined by *in situ* x-ray scattering and *ex situ* atomic force microscopy studies. This work is supported by the U.S. Department of Energy, Office of Science, under Contract W-31-109-Eng-38, and by the State of Illinois under HECA.

P6.51

INVESTIGATION OF THE LAYERED STRUCTURE OF POLYCRYSTALLINE DIAMOND THIN FILMS GROWN BY ECR-ASSISTED CVD BY SPECTROSCOPIC PHASE MODULATED ELLIPSOMETRY. S. Gupta, B.R. Weiner and G. Morell, Department of Physics, Univ. of Puerto Rico, San Juan, PR.

Polycrystalline diamond thin films grown on Si (111) by electron cyclotron resonance-assisted chemical vapor deposition (ECR-CVD) are examined using spectroscopic phase-modulated ellipsometry (SPME) from the near IR to UV range (830 nm-270 nm). By applying the conventional Bruggeman effective medium approximation (EMA) model and linear regression analysis (LRA) to the ellipsometry data, we obtained details about the film microstructure: (i) the multilayer structure and the effective thickness of the films; (ii) the volume fraction of the composites (sp³ C, sp² C) and of voids (%); (iii) the inhomogeneity of the structure along the growth axis and its variation with the seeding density; and, (iv) the surface roughness. Results obtained through ellipsometry modelling were compared with those obtained from other techniques. Micro-Raman spectroscopy was used to determine the relative sp³ C content in the films and their crystalline quality. Atomic force microscopy (AFM) measurements validated the estimated roughness found at around tens of nanometers. *This research work is supported from the Department of Energy (DoE Grant No. DE-FG02-99ER45796), and the University of Puerto Rico (UPR FIPI Grant No. 880244).

P6.52

EFFECT OF SULFUR ON CVD GROWTH OF DIAMOND (100). Hiroyuki Tamura, Hui Zhou, Seiichi Takami, Momoji Kubo and Akira

Miyamoto, Tohoku Univ, Dept of Material Chemistry, Sendai, JAPAN; Mikka N.-Gamo and Toshihiro Ando, National Institute for Research in Inorganic Materials, Ibaraki, JAPAN.

Diamond is expected to be the ultimate device material due to its extreme properties, e.g., the highest hardness, high thermal conductivity, and wide band-gap. A p-type semiconducting diamond is obtained by boron doping, which is expected to realize high speed and high power devices due to its high carrier mobility. Whereas, an n-type semiconducting diamond is difficult to obtain regardless many attempts using donor dopants (e.g., nitrogen and phosphorus), therefore, its development is crucial to realize the diamond devices. Recently, the n-type diamond has been obtained by chemical-vapor deposition (CVD) growth of (100) plane using CH₄/H₂/H₂S gas mixture [1], where sulfur is thought to be incorporated into the diamond lattice as a donor dopant. In the present study, the sulfur doping mechanisms into diamond (100) have been investigated using density-functional (DFT) calculations. The S atom is spontaneously inserted into the dimer bond on the diamond (100) and enhances CH₂ bridging across the trough. The further reactions to incorporate sulfur into the diamond lattice have been investigated. [1] I. Sakaguchi, M. N.-Gamo, Y. Kikuchi, E. Yasu, H. Haneda, T. Suzuki, and T. Ando, Phys. Rev. B, 60, 2139 (1999).

P6.53
ELASTIC PROPERTIES OF DIAMOND-LIKE AMORPHOUS CARBON FILMS GROWN BY COMPUTER SIMULATION OF ION-BEAM DEPOSITION PROCESS. Alexander Belov, Hans-Ulrich Jäger, Forschungszentrum Rossendorf e.V., Institut für Ionenstrahlphysik und Materialforschung, Dresden, GERMANY.

The unique mechanical properties of ta-C films such as high hardness and Young modulus are directly related to the atomic structure of amorphous carbon. Atomic-scale modeling is a valuable tool to study both growth mechanisms of amorphous carbon films and the properties sensitive to details of their structure, primarily to the content of sp³-bonded atoms. As it has been recently demonstrated, the steady-state growth of ta-C thin films can be modeled using the molecular dynamics method with realistic empirical interatomic potentials. It was shown that the experimentally observed high contents of sp³-bonded atoms (up to 90%) can be achieved using a potential function of Brenner with a slightly increased interaction radius. This provides a possibility to investigate the mechanical properties of amorphous carbon networks generated by a realistic growth process simulation, rather than by quenching the liquid carbon at high pressures as was done in previous studies. In this contribution we present results of the investigation of average and atomic-level elastic moduli of amorphous carbon networks with different sp³-contents, corresponding to C⁺ ion energies of E = 30-80 eV in the ion-beam deposition process. For the sake of comparison, the calculation of the elastic moduli was performed using not only the potential functions of Brenner, but also the potential function of Tersoff. The relaxational part of elastic moduli was computed using 3D-supercells with about 1000 atoms and an accurate iterative method for the solution of large linear systems. The elastic moduli tensor was found to show only small deviations from the elastic isotropy. Taking into account that the Brenner potential functions underestimate the bulk modulus of crystalline diamond, the results of computations are in an agreement with experimental measurements.

P6.54
DIRECT PATTERNING OF DIAMOND-LIKE CARBON BY MICRO-ELECTRODEPOSITION IN ORGANIC LIQUIDS. Hao Wang, Tomoaki Watanabe, Masahiro Yoshimura, Center for Materials Design, Tokyo Institute of Technology, Yokohama, JAPAN.

Direct patterning of diamond-like carbon in liquid phase has been achieved by a micro-electrodeposition method in organic liquids. Under a very high potential, with a thin metal wire electrode, the diamond-like carbon patterns with the diameter of about 5-10 μm have been directly formed on the Si wafer without any post-treatment. The composition and structure of deposits were verified by XPS and Raman spectroscopy. It is proposed that, when electrolysis of a solvent is carried out using a thin wire electrode, a local Joule heating might happen in the solvents, then under suitable conditions of energy dissipation, the glow discharge might happen if the applied voltage is sufficiently high. In this case, a very shallow primary reaction zone containing high concentrations of radicals originating from the solvent can be formed. Therefore, it can produce an extreme environment which is closely analogous to those brought about by plasma or ionizing radiation. This is to say, some non-equilibrium reactions may happen, or some metastable products may be obtained. This is the reason why the diamond-like carbon would form in liquids. Generally, the diamond or diamond-like carbon pattern has been made by gas phase technology with post-treatment, such as masking and removing mask after deposition. To our knowledge, this is the first time to report the direct patterning of diamond-like carbon without any

post-treatment, particularly in the liquid phase. This technology might be promising in the semiconductor industry.

P6.55
CHARACTERISTICS OF LASER-ABLATED PLASMA AND PROPERTIES OF DIAMOND-LIKE CARBON FILM IN PULSED LASER DEPOSITION. Yukihiko Yamagata, Tamiko Ohshima, Tomoaki Ikegami, Kenji Ebihara, Kumamoto Univ., Dept. of Electrical and Computer Engineering, Kumamoto, JAPAN; Ajay Sharma, Jagdish Narayan, North Carolina State Univ., NSF Center for Advanced Materials and Smart Structures, Raleigh, NC.

Diamond-like carbon (DLC) films have great potential for applications in mechanical and optical coatings, electronic devices, and field emitters. Pulsed laser deposition (PLD) has been employed to fabricate high quality DLC films with sp³ formation exceeding 80%. The mechanism of the PLD process, however, has not yet been well understood. Optical emission spectroscopy (OES) and laser-induced fluorescence (LIF) are powerful tools to diagnose the laser-ablated plasma, and are useful to establish correlation between plasma composition and properties of deposited films. In this paper, we describe systematic studies using OES^{1,2} and LIF on the plasma plumes generated from various kinds of carbon target. A KrF excimer laser was used to irradiate an amorphous carbon and a polycrystalline graphite targets. The optical emission spectra and the LIF signals were detected by a photomultiplier tube and an intensified CCD camera. In high vacuum, the emission lines of C⁺, C²⁺ and C³⁺ have been observed in addition to several atomic carbon lines in both targets. The emission intensity of C atoms increases with laser energy density increase. The 2-dimensional LIF measurements show that C₂ molecules locally exist near the target surface and the density decreases with laser energy density increase. Nanohardness of the deposited films decreases with the increase of the C₂/C emission intensity ratio, which is greatly influenced by the target crystallinity and the laser energy density. It is suggested that the C₂ molecule in the ablated plasma plume may not play an important role in producing high quality DLC films. 1. Y. Yamagata, A. Sharma, J. Narayan, R.M. Mayo, J.W. Newman, K. Ebihara, J. Appl. Phys. 86 (1999) 4154. 2. Y. Yamagata, A. Sharma, J. Narayan, R.M. Mayo, J.W. Newman, K. Ebihara, J. Appl. Phys. in press, (2000).

P6.56
HIGH RESOLUTION TRANSMISSION ELECTRON MICROSCOPIC STUDY OF HETEROEPITAXIAL NUCLEATION OF DIAMOND ON Ni THIN FILMS. W. Liu, R. Schlessler, J.T. Prater^a, Z. Sitar, Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC. ^a Army Research Office, RTP, NC.

Cross-sectional high-resolution transmission electron microscopy (XHRTEM) has been applied to investigate the interfacial microstructure formed during hot filament chemical vapor deposition (HFCVD) of oriented diamond on Ni thin films. A multi-layer structure with 100Å iridium and 1 μm nickel grown epitaxially on a MgO (100) wafer by electron-beam evaporation was used as a substrate. The 100Å Ir interlayer was used to overcome the delamination of Ni from the MgO substrate. Diamond was grown using a seeding and multi-step process.[1] Focused ion beam (FIB) technique was used for (TEM) sample preparation. Heteroepitaxial diamond nuclei formed at the early nucleation stage and after longer growth time were studied. A carbide interfacial layer between the diamond nuclei and Ni was observed. Diamond grew epitaxially on this interfacial layer with very few defects. All defects appeared to have propagated into the interfacial layer and consisted primarily of stacking faults and dislocations. The selected area diffraction showed a slight misorientation of the interfacial layer with the Ni film. It is believed, that the interfacial layer, which has the same crystal structure and a very close lattice constant with Ni, stabilized the sp³ carbon and facilitated diamond nucleation. A model describing the nucleation mechanism is proposed. [1]. P.C. Yang, R. Schlessler, C.A. Wolden, W. Liu, R.F. Davis, J.T. Prater and Z. Sitar, Appl. Phys. Lett. 70, 2960 (1996).

P6.57
INVESTIGATION OF THE OXIDATION BEHAVIOUR OF A TiALCRYN PVD HARD COATING. Mirkka I. Lembke, D. Brian Lewis, W.-Dieter Münz, Materials Research Institute, Sheffield Hallam University, Sheffield, UNITED KINGDOM; John M. Titchmarsh, Department of Materials, University of Oxford, Oxford, UNITED KINGDOM.

For dry high speed cutting oxidation resistance of the protective hard coating on the tool is very important. Therefore the effects of heat treatment on a TiAlN based hard coating deposited by a combined cathodic arc unbalanced magnetron sputtering technique have been studied using cross sectional transmission electron microscopy (XTEM) and energy dispersive X-ray analysis (EDX). The

combination of these techniques allowed to illustrate the diffusion paths and preferences in diffusion of various coating and substrate elements in a physical vapour deposited (PVD) type coating. The coating comprises a 2 μm thick TiAlCrYN coating on top of a 0.25 μm thick TiAlCrN base layer. In the as-deposited sample yttrium was uniformly distributed throughout the coating. The coating was heat treated at temperatures between 600°C and 900°C in air for 10h respectively. With increasing temperature the microstructure changed gradually from interrupted columnar growth to a fully columnar structure at 900°C as observed by XTEM. EDX analysis after heat treatment at 700°C showed the presence of substrate elements iron and chromium mainly at column boundaries in the base layer. In contrast no evidence of substrate elements could be observed in the TiAlCrYN coating thus showing a sharp change in elemental composition concerning chromium and iron between base layer and coating. This indicates that yttrium segregation in the TiAlCrYN coating along column boundaries inhibited column boundary diffusion of the substrate elements chromium and iron. EDX spectra taken at 800°C showed distinct segregation of yttrium along the column boundaries. The substrate elements, iron and chromium were observed through the coating along column boundaries up to 0.75 μm from the base layer/ coating interface. After heat treatment at 900°C the substrate elements had diffused from the substrate/ coating interface to the coating surface. Yttrium out-diffused, too and was located nearby TiO₂ crystals in the oxide layer.

SESSION P7: DIFFUSION AND MORPHOLOGICAL
EVOLUTION OF SURFACES AND THIN FILMS
Chair: Woei Wu (Larry) Pai
Wednesday Morning, November 29, 2000
Room 302 (Hynes)

8:30 AM *P7.1

JOINT SCANNING TUNNELING MICROSCOPY AND QUARTZ CRYSTAL MICROBALANCE STUDY OF SLIDING FRICTION AND DIFFUSION IN ADSORBED MOLECULES. J. Krim, B. Borovsky, B.L. Mason and S. Winder, North Carolina State University, Department of Physics, Raleigh, NC.

Energy transfer plays an important role in many surface processes such as surface diffusion, vibrational relaxation and sliding friction in adsorbed molecules. The Quartz Crystal Microbalance (QCM) has in recent years been employed to reveal much fundamental information on the phononic and electronic energy dissipation mechanisms associated with the sliding of atomically thin films along surfaces, a phenomenon closely related to the spreading diffusion of a film on its substrate.[1] While in quantitative agreement with theory and computer simulation, the QCM data have not been cross-referenced to scanning probe measurements of sliding friction and diffusive behavior of atoms along surfaces. We have thus combined a STM and QCM to allow direct imaging of films adsorbed on the QCM electrode under both stationary and oscillating conditions.[2] The results of these studies will be described, along with a discussion of whether our current knowledge of the fundamentals of friction is sufficient to enable motional control of adsorbates on surfaces through frictional drag forces.

Supported by NSF and AFOSR

[1]A. Widom and J. Krim, Phys. Rev. E, 49, 4154 (1994) [2]B. Borovsky, B.L. Mason and J. Krim, submitted to J. Appl. Phys. (2000)

9:00 AM P7.2

SURFACE SMOOTHING CONTROLLED BY DIRECT EXCHANGE WITH BULK VACANCIES IN NiAl. K.F. McCarty, J.A. Nobel, N.C. Bartelt, Sandia National Laboratories, Livermore, CA.

We have examined the kinetics of island decay on the NiAl (110) surface using low-energy electron microscopy (LEEM). Remarkably, the decay rates are constant in time and totally independent of the local environment (e.g., the width of the immediately adjacent terraces and degree of island curvature). Given the lack of surface current between islands of different curvature, we conclude that surface diffusion is not important to the smoothing process. Instead, we find unambiguous evidence that bulk vacancies are responsible – we visibly observe exchange between bulk vacancies and the surface when the sample temperature is changed. For a temperature increase, the surface steps advance. For a temperature decrease, the surface steps recede. These changes result from the increase (decrease) in bulk vacancy concentration for a temperature increase (decrease). Remarkably, the size change accompanying a temperature change is strictly proportional to the perimeter (step length) of the island, and again is totally independent of the local environment. Thus, we conclude that the atoms at surface steps undergo direct exchange with bulk vacancies. We will present simple mathematical models showing how this mechanism quantitatively describes the constant-rate

kinetics as well as the bulk-derived flux associated with a temperature change. The complete independence of the surface dynamics on the local environment results from the fact that the steps are interacting directly with the bulk, and thus, the local step density and curvature are largely irrelevant. This work was performed under the U.S. Department of Energy contract DE-AC04-94AL85000 and supported by the Office of Basic Energy Sciences-Division of Materials Sciences.

9:15 AM P7.3

STM CHARACTERIZATION OF Cu THIN FILMS GROWN BY DIRECT ION DEPOSITION. J.M. Pomeroy, A. Couture, J.

Jacobsen¹, J.P. Sethna, B.H. Cooper², J.D. Brock; Cornell Center for Materials Research, ¹currently with Haldor Topsoe A/S, Denmark ²deceased August 9, 1999.

In certain cases, the incidence energy of constituent atoms activates an atomistic insertion mechanism, which decreases the surface roughness of metal thin films. In an effort to probe this effect, homoepitaxial copper films were grown using a mass/energy selected direct ion deposition technique that allows precise control of the incidence energy. Surface roughness is measured using an STM within the same UHV surface analysis system. The activation of the insertion mechanism near 20 eV triggers smoother crystal growth until the beneficial effects are obscured by adatom/vacancy creation near 30 eV. A sophisticated kinetic Monte Carlo/molecular dynamics (KMC-MD) model supports this interpretation.

9:30 AM P7.4

THERMAL DECAY OF ISOLATED SINGLE Si MOUNDS ON THE Si(100)2 \times 1 SURFACE. Ayahiko Ichimiya, Masashi Suzuki and Shunsuke Nishida, Nagoya Univ, Dept of Quantum Engineering, Nagoya, JAPAN.

Silicon mounds formed on the Si(100)2 \times 1 surface have been observed by STM at substrate temperature of 500°C. The mound has been fabricated by an STM tip. The shape of the mound is a quadrangular pyramid with facets of regular array of steps with double layer height. For the all step, the dimer rows are perpendicular to the step edges, so called the D_B step. Just after the fabrication, the pyramid begins to decay immediately layer-by-layer. During the decay, area of the bottom single layer of the pyramid is grown toward the dimer row direction which is perpendicular to the S_B steps. The layer width does not change toward perpendicular to the dimer rows parallel to the S_A steps. The area of the topmost layer of the pyramid decreases toward perpendicular to the dimer rows, because the both S_B step edges are pinned by the step edges of the lower ones. Therefore the D_B step edges remain at the each one. During decay, the D_B steps move scarcely, but only the S_B steps at the bottom layer move due to attachment and detachment of atoms which are detached from the upper layers. Therefore the D_B and S_A steps are permeable. The decay process of a single layer mound on the Si(100) surface is very different from that of the topmost layer of the pyramid. The S_B steps are fluctuate very much and kinks of the S_A steps are also moving. The aspect ratio of the mound oscillates between about 2.5 and 1.5. This means that detached atoms at the S_A step edges are attached at S_B step edges when the ratio becomes smaller than a certain value. The decay process of the topmost layer of the pyramid might be explained by this detachment and attachment behavior of the single layer mound.

9:45 AM P7.5

ADATOM KINETICS ON AND BELOW THE SURFACE: THE EXISTENCE OF A NEW DIFFUSION CHANNEL. J. Neugebauer, T.K. Zywiets, M. Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, GERMANY; J.E. Northrup, Xerox Palo Alto Research Center, Palo Alto, CA; H. Chen, and R.M. Feenstra, Carnegie Mellon Univ., Pittsburgh, PA.

The surface migration of adatoms strongly affects the epitaxial growth mode and thus the quality of the material. For semiconductors, it is generally assumed that the most efficient diffusion channel for adatoms is *on the surface*, i.e., the diffusing atom remains above the top surface layer of the substrate. Subsurface diffusion is regarded as less efficient or negligible since (i) adatoms in subsurface sites are expected to be less stable than in on surface sites and (ii) surface diffusion is significantly faster than bulk diffusion. Employing density-functional theory calculations we have identified a mechanism which opens a novel and very efficient subsurface diffusion channel. The system we will focus on is the GaN(0001) surface, where, in the very Ga-rich conditions optimal for growth, a metallic laterally contracted bilayer of Ga is stable.[1] A metallic adlayer structure is also stable if In is deposited on the surface: an In adlayer structure is energetically favorable over a wide range of growth conditions. These metallic adlayer structures strongly affect the adsorption sites, the migration paths, and the diffusion barriers. For the In adlayer structure we show that the stable adsorption site for N adatoms is *inside the metallic double layer* and that adatoms diffuse between

these two layers. The calculated diffusion barrier for subsurface diffusion is 0.5 eV, compared to 1.3 eV for on surface diffusion [2]. Thus, the stability of a metallic double layer opens an unexpected subsurface diffusion channel that strongly *enhances the mobility for N adatoms*. Based on these results we discuss whether and how this effect may be utilized to improve GaN growth. [1] J. E. Northrup, J. Neugebauer, R.M. Feenstra, and A.R. Smith, Phys. Rev. B **61**, 9932 (2000). [2] T. Zywietz, J. Neugebauer, and M. Scheffler, Appl. Phys. Lett. **73**, 487 (1998).

10:15 AM *P7.6

SURFACE FLUCTUATIONS AND STABILITY OF NANOSCALE STRUCTURES. Ellen D. Williams, K. Thuermer, J. Reutt-Robey, T.L. Einstein, C. Gupta and R. Ramesh, Materials Research Science and Engineering Center, University of Maryland, College Park, MD; A. Ichimiya, K. Hayashi, M. Uwaha, K. Watanabe, Nagoya University, Furo-Cho, Chikusa-ku, Nagoya, JAPAN; A. Emunds and H.P. Bonzel, Institut für Grenzflächenforschung und Vakuumphysik, Forschungszentrum Jülich, Jülich, GERMANY.

As the size of material elements approaches the nanoscale, structural fluctuations at even the scale of a single atom can affect the material properties. Such fluctuations are most likely to occur at low-dimensional boundaries such as steps or domain boundaries, and also serve as the rate limiting process in the decay or evolution of nanostructures. In this talk, three examples where simple boundary fluctuations can be related to complex structural evolution will be presented. The decay of metastable cones of silicon, of 10-20 nm base diameter, has been observed using scanning tunneling microscopy. Despite the faceted edges of the cones, the decay occurs by sequential removal of layers of material. The rate of the decay is quantitatively recovered by considering the dominant driving force to be the curvature driven shrinkage of the layers. The reshaping of lead crystallites after a temperature jump has been observed using variable temperature scanning tunneling microscopy. Facet growth occurs by layer removal and redistribution of the mass to the edges of the crystallite. The balance of the curvature of the edges of the shrinking layers with the chemical potential change induced by the temperature jump provides a quantitative description of the structural evolution. The evolution of ferro-electric domains in lead zirconate titanate thin films has been observed using piezo-response scanning electric force microscopy. Here the curvature and pinning of the edges of the domain boundaries in competition with the depolarizing field governs the kinetics of the decay process. The kinetics of the evolution of a single domain surprisingly is identical to the depolarization kinetics of the macroscopic film, providing an immediate path to understanding polarization retention. *Work supported by the UMD-NSF MRSEC.

10:45 AM P7.7

ROUGHENING DUE TO EDGE DIFFUSION FOR IRREVERSIBLE AGGREGATION. C. Ratsch, M. Kang, M.C. Wheeler and R.E. Caflisch, UCLA, Los Angeles, CA; M.F. Gyure, HRL Laboratories, Malibu, CA.

We develop an island dynamics model that employs the level-set technique to describe epitaxial growth. Island boundaries for islands in the n th layer are defined by the set of curves $\varphi = n$, where φ is the so-called level-set function. The island boundaries evolve with a velocity that is obtained from solving the diffusion equation for the spatially varying adatom concentration on the surface. Edge diffusion is incorporated by including a curvature dependence. We find that an increase in edge diffusion enhances surface roughening for a model of irreversible aggregation. Our result is confirmed by KMC simulation with edge diffusion as an additional microscopic parameter. The reason for this effect is the following: Faster edge diffusion makes the islands more compact, leading to a significant adatom concentration on top of islands at earlier times. As a consequence, nucleation in higher layers occurs faster, increasing the surface roughness.

11:00 AM P7.8

STEP WANDERING ON SURFACES WITH MULTIPLE STRUCTURAL PHASES DURING GROWTH. Hiroki Hibino, Yoshikazu Homma, Toshio Ogino, NTT Basic Research Labs, Kanagawa, JAPAN; Changwu Hu, Ignatius S.T. Tsong, Arizona State Univ, Dept of Physics and Astronomy, Tempe, AZ; Makio Uwaha, Nagoya Univ, Dept of Physics, Nagoya, JAPAN.

Two kinds of instabilities of steps during step-flow growth have been intensively studied; step bunching and step wandering. These instabilities are due to the asymmetry in the incorporation of atoms to the step from the upper and lower sides. Typical causes of the asymmetry are the Ehrlich-Schwoebel effect and the drift of adatoms by an external field. In this paper, we demonstrate that the step wandering occurs on surfaces with multiple structural phases, and that the asymmetric atom incorporation is caused by the difference in the mass transport on the different phases. We first observed step configurations on Si(111) after Si growth using *ex situ* AFM and

in situ UHV-SEM. The step configuration after growth dramatically changed around the phase transition temperature between 1×1 and 7×7 . After 20-nm-thick Si layers were grown, steps remained fairly straight on the surface covered with only 1×1 or 7×7 . However, on the surface where 1×1 and 7×7 coexisted, step wandering occurred. In order to clarify the mechanism, we next observed the change in step shape during the initial growth stages directly using LEEM. On the surface with both 1×1 and 7×7 , the steps preferred to protrude at the position in contact with 1×1 . This suggests that more atoms diffuse to the step through 1×1 than 7×7 . During the phase transition, the terraces on the upper and lower sides of the step are mainly covered with 7×7 and 1×1 , respectively. Therefore, the difference in the mass transport on 1×1 and 7×7 causes the asymmetric atom incorporation. Thus, the step wandering occurs during growth. Reconstructive phase transitions often start at steps, and adsorbate-induced reconstructions often decorate one side of the step. The mass surface diffusion coefficient should depend on the surface structure. The step wandering and/or step bunching could occur on various multi-structural systems.

11:15 AM P7.9

WHY IS KPZ TYPE SURFACE ROUGHENING SO HARD TO OBSERVE? Jason T. Drotar, Y.-P. Zhao, T.-M. Lu, G.-C. Wang, Rensselaer Polytechnic Inst, Dept of Physics, Applied Physics, and Astronomy, Troy, NY.

The Kardar-Parisi-Zhang (KPZ) surface roughening model was proposed almost fifteen years ago. Although there has been a large number of theoretical studies, there are almost no examples of thin film evolution obeying the KPZ equation. KPZ-type surface roughening requires that the flux of incoming particles remain spatially constant at the surface, so that the growth rate does not vary across the film surface. In other words, the growth must be conformal. One would expect KPZ-type growth in a chemical vapor deposition (CVD) process, since the CVD growth is usually conformal. This can be achieved in the ballistic transport regime with small sticking coefficients. We construct a non-local, KPZ-like growth model by considering the effect of surface re-emission. Our Monte Carlo simulations show that, if we assume that the sticking coefficients for different orders of re-emission are the same, the growth will change from shadowing growth (column formation) to KPZ-type growth when the sticking coefficient varies from one to zero. However, in practice, the sticking coefficient can vary with order of re-emission due to complicated precursor-substrate interactions, such as thermal accommodation and inelastic collisions. Our simulations show that for different orders of re-emission, different kinds of roughening behavior appear. Furthermore, in our simulations, the growth may look close to conformal even under conditions that give roughening exponents different from those of the KPZ equation. Therefore, to achieve KPZ-type growth in a low-pressure CVD process, one requires a very stringent condition, which usually is not experimentally feasible. Work supported, in part, by NSF.

11:30 AM P7.10

HETEROEPITAXIAL GROWTH MODE TRANSITIONS IN THE PRESENCE OF A SCHWOEBEL BARRIER AT AN ISLAND EDGE. Vladimir I. Trofimov, Vladimir G. Mokerov, Inst of Radioengr & Elec of RAS, Dept of Nanoelectronics, Moscow, RUSSIA.

Recently developed model [1] for homoepitaxial growth on a singular surface in the presence of a Schwoebel barrier at an island edge is extended to the case of heteroepitaxy (without lattice mismatch) by introducing two different adatom mobilities in the first layer (heterodiffusion) and in all the next layers (self-diffusion). Model consists of an infinite set of the rate equations for areal densities of adatoms and 2D islands, and coverage in successive growing layers and contains several numerical parameters, characterizing the surface mobility of adatoms, critical nucleus size and stability, Schwoebel effect, and growth coalescence behaviour. Systematic studies of the growth behaviour depending on these parameters are performed with a focus on the transient growth regimes: layer-by-layer (LL) to smooth multilayer (SML) and SML to rough 3D growth. It is shown that the effect of "heteroepitaxy" (two adatom mobilities) confined of course within several first layers, is strongly dependent on the barrier height and relative difference between hetero- and self-diffusion coefficients. The lower heterodiffusion coefficient relative to that of self-diffusion leads to smoother growth and thus retards the LL-SML growth transition, while the higher heterodiffusion coefficient leads to a rougher growth and assists to that transition and especially to SML-3D growth at higher Schwoebel barriers. We studied also the nucleation kinetics in successive layers of which unlike to a first layer a little is known. We show that in a smooth growth regime (LL and SML) after deposition about 5-10 monolayers it acquires an universal scaling form and corresponding exponents are determined. [1] V.I. Trofimov, V.G. Mokerov, Comput. Materials Science 17 (2000) 510

SESSION P8: QUANTUM DOTS AND QUANTUM SIZE EFFECTS

Chair: Jian N.M.N. Shen
Wednesday Afternoon, November 29, 2000
Room 302 (Hynes)

1:30 PM *P8.1

ELECTRONIC PROPERTIES OF SELF-ORGANIZED, ONE-DIMENSIONAL METAL WIRES ON Si(111). Eli Rotenberg, C.M. Lee, Lawrence Berkeley Natl. Lab; J. Schaefer, S.D. Kevan, Department of Physics, Univ. of Oregon; H.W. Yeom, Dept. of Physics, Yonsei Univ.; I. Matsuda, T. Ohta, Dept. of Chemistry, Univ. of Tokyo; S. Takeda, K. Horikoshi, T. Nagao, S. Hasegawa, Dept. of Physics, Univ. of Tokyo, Tokyo, JAPAN.

An exciting current topic in condensed-matter physics is the role of correlation effects and many body interactions in low-dimensional metallic systems. These systems demonstrate the inherent instability of metals to non-metallic ground states, which becomes more likely as the dimensionality of the systems is reduced. Of further interest is the application to future technological devices such as nanowires. One of the most promising routes to the study of the fundamental physics of these systems is the creation and in situ analysis of self-organized one-dimensional metal wires on Si. These systems have a very high degree of one-dimensional character and have been shown to display classic one-dimensional effects such as Peierls distortion and Luttinger liquid behaviour. One of the best techniques to analyze these systems is angle-resolved photoemission, which can directly measure the momentum-resolved electronic density of states. We present results for two model systems: 3×1 Ba/Si(111) [1] and 4×1 In/Si(111) [2], two metal adsorbate systems which self-organize into one-dimensional chains. Applying angle-resolved photoemission to single-domain samples, we demonstrate the electronic bands have strict one-dimensional character in momentum space (within our experimental uncertainty). Contrary to expectations from electron-counting arguments, the Ba/Si system is a correlated insulator and shows a signature of spin-charge separation. At RT the In/Si system is metallic; however, it exhibits evidence of a Peierls distortion to 4×2 symmetry at low temperature. [1] J. Schaefer, E. Rotenberg, and S. D. Kevan, submitted. [2] H.W. Yeom, S. Takeda, E. Rotenberg, I. Matsuda, K. Horikoshi, J. Schaefer, C.M. Lee, S.D. Kevan, T. Ohta, T. Nagao, and S. Hasegawa, Phys. Rev. Lett. 82 (24), 4898 (1999).

2:00 PM P8.2

DISPERSION OF QUANTUM-WELL STATES IN ULTRATHIN Al FILMS ON Si(111). Lucia Aballe¹, Celia Rogero¹, Shubba Gokhale^{1,2} and Karsten Horn¹. ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, GERMANY. ²Physics Department, University of Pune, Pune, INDIA.

Studies of quantum-well phenomena in thin metal films have so far concentrated on the noble metals, largely unreactive with many substrates. Here we report investigations of the thickness-dependent electronic structure of aluminium films on Si(111)7x7 using angle resolved photoemission. Deposition at 100K induces an abrupt and homogeneous interface and leads to the growth of an epitaxial, two-dimensional Al(111) overlayer of good crystalline quality. We assign this to reduced diffusion and more homogeneous nucleation during the first stages of film growth. Even after annealing to room temperature and above, the films are highly stable and improve their crystalline order while retaining their 2D character, and the interface remains homogeneous, in contrast to the films grown directly at room temperature. The high quality of films deposited at low temperature permits the observation of overlayer states for thickness up to 30 Al monolayers. The experimental dispersion of these quantum-well states in the surface Brillouin zone can be well explained in terms of the Al band structure. However, a more detailed analysis reveals the intriguing effect of the Si band structure on peak positions and lineshapes. The substrate's electronic structure largely determines the energy-dependent phase shift of the electron waves at the Al/Si interface, and thus its signature becomes apparent in the data, making possible the mapping of the band edges through the induced changes. The importance of this observation lies in its ground state character: no optical transition is involved in determining substrate band edges, since the Bloch electrons of the overlayer are used for probing the interfacial structure. This observation clearly demonstrates that the details of the substrate electronic structure need to be taken into account for a complete analysis of the dispersion of metallic quantum-well states.

2:15 PM P8.3

CAPPING AND ORDERING OF InAs QUANTUM DOTS ON GaAs(001). J. Falta, Th. Schmidt, Institute for Solid State Physics, Bremen, GERMANY; K. Zhang, Ch. Heyn and W. Hansen, Institute for Applied Physics, Hamburg, GERMANY.

We have performed measurements of grazing incidence x-ray small angle scattering (GISAXS) and grazing incidence x-ray diffraction (GIXRD) on InAs quantum dots on GaAs(001). The quantum dots were grown by molecular beam epitaxy (MBE) at 450°C. After InAs deposition, AFM studies performed ex situ show that the quantum dots are well defined in size with an average diameter of 30 ± 10 nm. Employing GISAXS for these samples, we find a preferential ordering of the quantum dots array in [110] and less pronounced in [1-10] surface direction. In these directions first and second order satellite peaks are observed in GISAXS, corresponding to an average dot separation of about 64 nm and a dot-dot correlation length of approximately 100 nm. Comparative measurements were performed for InAs quantum dot arrays which have been capped by a GaAs layer. These show GISAXS spectra of much less pronounced structure. This indicates a loss of ordering during the growth process of the capping layer which we attribute to intermixing of GaAs and InAs during GaAs deposition. For the uncapped InAs quantum dot arrays additional facet spots are observed for in-plane scattering conditions. These allow to determine the shape of the dots. Under our growth conditions, we find the dots to consist of an octagonal base with {111} and {101} side facets. GIXRD shows a partial relaxation of the InAs with a wide distribution of the local lattice constant but an almost vanishing fraction of fully strained InAs. The extent of Ga intermixing into the InAs quantum dots can be estimated to be smaller than 3% volume fraction. For the capped quantum dots however, no InAs peak can be found in GIXRD pointing to a strong intermixing of InAs and GaAs during growth of the capping layer.

2:30 PM P8.4

ORGANIZATION OF SELF-ASSEMBLED QUANTUM DOTS IN SiGe/Si MULTILAYERS: EFFECTS OF STRAIN AND SUBSTRATE CURVATURE. P. Sutter, E. Mateeva, Colorado School of Mines, Golden, CO; L. Vescan, Institut für Schicht und Ionentechnik, Forschungszentrum Jülich, Jülich, GERMANY.

The formation of three-dimensional (3D) islands by stress-driven self-assembly in heteroepitaxial growth has been studied as a possible way of creating large-scale arrays of quantum dots. The proposed use of such epitaxial quantum dots in electronic devices would require a narrow size distribution of the dot ensemble and its organization into a long-range ordered array. Epitaxial multilayer structures, in which layers with self-assembled islands (e.g., consisting of a SiGe alloy) alternate with spacer layers composed of the substrate material (e.g., Si), have been used to control both the island size distribution and spatial organization¹. Nonuniform strain on the planar spacer surface was identified as the driving force for the observed improved ordering in such multilayer structures². In addition to surface strain, any curvature of the spacer surface will also strongly affect the formation of the next layer of 3D islands. We have used transmission electron microscopy to systematically study the competition between strain and curvature effects in organizing SiGe island on Si(001). Our results show that unique island configurations - some of which are promising for application in quantum devices - can be achieved by controlling both strain and curvature of the spacer surface. 1. E. Mateeva, P. Sutter, J.C. Bean, and M.G. Lagally, Appl. Phys. Lett. 71, 3233 (1997). 2. J. Tersoff, C. Teichert, and M.G. Lagally, Phys. Rev. Lett. 76, 1675 (1996).

2:45 PM P8.5

QUANTUM WELL PHOTOEMISSION SPECTROSCOPY OF ATOMICALLY UNIFORM FILMS. J.J. Paggel, Institut fuer Experimentalphysik, Freie Universitaet Berlin, GERMANY; T. Miller, D.-A. Luh, and T.-C. Chiang, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana, IL.

Angle resolved photoemission is a well-suited tool for the investigation of the electronic structure of materials. However, precise determination of the ground state electronic structure and the lifetime of the valence hole by traditional band mapping are obscured by the physics involved in the photoemission process itself. The observed peak width of the direct transition peak not contains information on the lifetime of the photo hole, including electron-phonon coupling, but also contributions from the band dispersion of the initial state, sample inhomogeneities, and most prominently the lifetime of the final state of the photoemission process. All final state contributions are easily removed by performing photoemission from a two-dimensional system, such as surface states, as widely demonstrated in the literature. Electron states confined in thin films also qualify as two-dimensional electron states, and in general should lead to narrow photoemission peaks, largely simplifying data analysis for the investigation of bulk electronic structure. Here data analysis is complicated by a possible error in film thickness, as well as possible thickness fluctuations across the sample. By employing a low temperature deposition and annealing technique for the growth of Ag on Fe(100) whisker samples, we are able to produce films of Ag, perfect enough that experiments on uniform films are possible. The high quality films allow the

observation of quantum well features in the sp-band and the d-band of Ag as function of film thickness. The signal from individual atomic layers is detectable, even fractions of monolayers generate unique signatures in the spectra. The observed spectral features are analyzed with respect to the line shape and peak position as function of temperature, emission angle, and photon energy employed in the experiment, leading to detailed information on the electronic band structure of Ag.

3:30 PM *P8.6

QUANTIZED CONDUCTANCE OF METAL POINT CONTACT.
Kunio Takayanagi, Tokyo Institute of Technology, Dept of Materials Science, Yokohama, JAPAN.

Quantized point contact (QPC) formed between two metal electrodes attracts much interest from fundamental physics and device technology, because of conductance quantization at room temperature. Conductance quantization occurs when the nanowire formed at QPC has diameter of the scale of Fermi wave length of electrons. We investigated conductance and structure of gold QPC by transmission electron microscopy with STM geometry. Following to our recent studies, topics on QPCs are reported and discussed: (1) structure of gold QPC and conductance, (2) magic structure of gold nanowire at QPC, (3) fractional conductance of QPC and temperature effect, (4) non-linear behavior of QPC and quantum diode. The work was done partly at Takayanagi surface ERATO project at Japan Science and Technology.

4:00 PM P8.7

DISPERSION AND QUANTUM CONFINEMENT OF ANISOTROPIC Ag(110) SURFACE STATES AT STEPS.
J.I. Pascual, Z. Song, J.J. Jackiw, H. Conrad, K. Horn, H.-P. Rust. Fritz-Haber-Institute der Max-Planck-Gesellschaft, Berlin, GERMANY.

Here we present the first dispersion measurements with Scanning Tunneling Spectroscopy of surface states (SS) centered at a Brillouin Zone boundary: the \bar{Y} point in Ag(110). With a 4K-STM we analyse the oscillations in the charge density as the SS wave functions scatter off step edges. Contributions from two SS in the energy range from the Fermi level E_F up to the vacuum level are resolved. These SS have their lowest energy at the BZ boundary (\bar{Y}). The states at this energy have a one-dimensional character, and they propagate for long distances. Our evaluation of the $E(k_{\parallel})$ dependence shows that the bands exhibit an approximately parabolic dispersion, affected at high energies by the continuum of bulk bands near the Γ point. The reflection properties of atomic steps on Ag(110) are investigated by analysing the interference patterns of the SS confined in the region between two [100] step edges. Here, the quantum confinement discretises the dispersion curve, and only standing waves are permitted. We find that the scattering properties of steps depend on the width of their neighbour terraces through the interference between the reflected and transmitted component of standing waves at each side. Modification of the dispersion relations at narrow terraces will be also analysed.

4:15 PM P8.8

DIRECT PHOTOEMISSION FROM IMAGE POTENTIAL STATES OF Ag (111) FILMS GROWN ON WSe₂ BY VAN DER WAALS EPITAXY. Christian Pettenkofer, Hahn-Meitner-Institut, Berlin, GERMANY; Andreas Otto, IPkM, Heinrich-Heine-Universität Düsseldorf, GERMANY.

Layered compounds of the transition metal dichalcogenides facilitate the epitaxial growth of heterocontacts despite a large lattice mismatch. Films grow azimuthally ordered with their own lattice constant on the hexagonal (0001) substrate. The electronic properties of the junction turned out to be ideal, they seem to follow despite a small correction due to interfacial dipoles the electron affinity rule, which is explained by the nonreactive and inert interface of the layered compounds, exposing no dangling bonds at the contact plane. Ag grows on the (0001) so called van der Waals plane of WSe₂ azimuthally ordered islands exposing a clean (111) surface to vacuum. Accordingly a LEED pattern showing the 3-fold symmetry of Ag (111) is superimposed on the 6-fold WSe₂ pattern. In STM nicely ordered islands of equal height and lateral dimensions of about 70nm are resolved. The Shockley type surface state S1 of clean Ag (111) is observed in photoemission with 21 eV in normal emission. At the Schottky barrier a nonequilibrium surface photo voltage is generated by the 21eV photons recognizable by a shift of the Ag emissions with respect to the substrate. By excitation with photon energies in the range of 3.8-5 eV strong electron emission below the threshold (as determined by the macroscopic work function of Ag(111) and the substrate) is observed which is attributed to a resonant excitation of electrons from S1 into image states n=1 and n=2 of the Ag (111) as a final state. An emission due to 2PPE is ruled out. Tentatively we explain the subthreshold emission due to the formation of a triple

junction at the Schottky barrier Ag/WSe₂ interface. Electrons resonantly excited to image states n=1 and n=2 above a Ag (111) oriented island may escape at the edge of the island into vacuum.

4:30 PM *P8.9

CRITICAL THICKNESSES AND QUASIPERIODIC SUPERSTRUCTURES OF ULTRATHIN Ag OVERLAYERS ON (110) SURFACES OF III-V SEMICONDUCTORS. Ph. Ebert, Institut fuer Festkoerperforschung, Forschungszentrum Juelich, Juelich, GERMANY and Dept. of Physics, University of Texas, Austin, TX; C.K. Shih, Dept. of Physics, University of Texas, Austin, TX.

Ultrathin and atomically flat metal overlayers can be grown on many semiconductor substrates using a two-step growth procedure at low temperatures, despite the frequently preferred three-dimensional growth mode at elevated temperatures. We present here the structure and properties of Ag films on (110) surfaces of III-V semiconductors obtained by deposition of Ag at 135 K followed by annealing at room temperature. Scanning tunneling microscopy images and low-energy electron diffraction pattern show that Ag films obtained on Ga-V semiconductors are all well ordered, atomically flat, and exhibit specific critical thicknesses, which are a function of the substrate material. In contrast, Ag films on In-V semiconductors are increasingly disordered, although they are still very flat compared to films grown at elevated temperatures. The (111) oriented Ag films on III-arsenides and III-phosphides exhibit two-fold superstructures, whereas on III-antimonides threefold structures were found. Only for Ag films on GaAs(110) substrates we found a one-dimensional quasiperiodic superstructure independent of the thickness of the film. This exceptional structure provided us with a model system for investigations of the properties of one-dimensional quasiperiodic systems. In particular, we investigated the disorder as well as the structural defects and identified that the system can be described well by a Fibonacci sequence with deviations due to dislocations, phason defects, and domain walls. The effect of different substrates on the critical thicknesses, morphology, and structure of the Ag films will be explained within the framework of the electronic growth mechanism. In addition, the influences of substrate lattice and the chemical structure at the interface will be evaluated. This work has been done in collaboration with K.-J. Chao, Zhenyu Zhang, Q. Niu, H. Yu, and C.-S. Jiang.

SESSION P9: INSULATING, ORGANIC, AND CATALYTIC SURFACE STRUCTURES

Chair: Ellen D. Williams
Thursday Morning, November 30, 2000
Room 302 (Hynes)

8:30 AM *P9.1

NANOASSEMBLED MODEL CATALYSTS: CHANGING EFFICIENCY AND SELECTIVITY ATOM BY ATOM. Ulrich Heiz, University of Lausanne, IPMC, Lausanne, SWITZERLAND.

Cluster-assembled materials open fascinating new routes for tuning physical and chemical properties by changing cluster size and often these materials behave completely differently than their bulk analogues. By depositing gas phase cluster cations on various oxide surfaces, cluster model catalysts are fabricated, which exhibit remarkable catalytic activity. While inert as bulk material, gold cluster catalysts oxidize carbon monoxide with Au₈ to be the smallest active size. In contrast to the high selectivity of Pd(111) surfaces for the cyclotrimerization of acetylene, small supported Pd_n clusters reveal a strongly size-dependent selectivity for the polymerization of acetylene and catalyze the cyclotrimerization as well as the hydrogenation of the formed intermediate C₄H₄.

9:00 AM P9.2

X-RAY CRYSTAL TRUNCATION ROD STUDIES OF THE REVERSIBLE SURFACE TRANSFORMATION OF THE [001] CRYSTAL SURFACE OF LaAlO₃. Robin J. Francis, Simon C. Moss, Allan J. Jacobson, University of Houston, Houston, TX; Hubert Zajonz, Doon Gibbs, Brookhaven National Laboratory, Upton, NY.

LaAlO₃ is a perovskite oxide extensively used as a substrate for superconductor thin film growth. Previous observations¹ had suggested a reversible change in the surface stoichiometry of LaAlO₃ between room temperature and 250°C, but no direct structural information was available. We have studied the surface structure of [001] oriented single crystals of LaAlO₃ using crystal truncation rod (CTR) analysis, a technique capable of providing such information. We have recorded CTR profiles in a number of different lattice directions at room temperature and above 300°C to study in detail the temperature dependence of the surface composition and structure. A combination of least squares fitting and simulated annealing techniques have demonstrated that at room temperature the surface of LaAlO₃ is aluminum terminated and that a fairly minor structural rearrangement of surface layers relative to the perfectly cut surface

occurs, mostly involving movement of the oxygen atoms out of the surface layer and a concomitant (although smaller) movement of the aluminum atom into the bulk. At high temperature there is a much more radical structural change. In particular, the aluminum atoms in the surface move a considerable distance into the bulk (0.18 of a unit cell) changing from a five coordinated position to a pseudo-tetrahedral site. This is accompanied by fairly substantial movements of the oxygen atoms in the top two surface layers. While the lanthanum atom does not move to such a degree, a small movement towards the surface can clearly be discerned from the CTR data. This change is found to be fully reversible; on changing back to room temperature the structural reconstruction reverses and the surface structure reverts to its previous state.

This work is supported by the NSF/MRSEC program DMR-9632667. ¹J. Yao, P.B. Merrill, S.S. Perry, D. Marton, J.W. Rabalais, Journal of Chemical Physics 108, 1645, (1998).

9:15 AM P9.3

STRAINED EPITAXIAL GROWTH AND PRECURSOR-INDUCED STRUCTURAL RELAXATION OF ORGANIC FILMS: PTCDA ON Ag(111). M. Sokolowski, Institut für Physikalische und Theoretische Chemie, Universität Bonn, GERMANY; L. Kilian, E. Umbach, Experimentelle Physik II, Universität Würzburg, Am Hubland, Würzburg, GERMANY.

Highly ordered films of organic molecules on inorganic substrates are presently subject for investigations aiming at improved properties of organic electronic devices. Organic molecular beam epitaxy (OMBE) has proved to be one of the most attractive routes to achieve films of high structural quality. However, since molecule-substrate interaction may overweight molecule-molecule interaction by far this may lead to highly ordered, but strongly strained films with structures commensurate with the substrate surface. Perylene-tetracarboxylic-dianhydride (PTCDA) films have been investigated on different substrates. On Ag(111) the bonding at room temperature (RT) is site specific and yields a commensurate long-range ordered monolayer that is very similar (2% misfit) to the (102)-plane of β -phase PTCDA. Significant differential chemical shifts in UPS and NEXAFS reveal that the bonding is chemisorptive. However, films grown at low substrate temperature (< 160 K) show different electronic spectra, which transform into the RT spectra upon annealing. This indicates the adsorption of PTCDA in a metastable, chemisorptive precursor state at low temperatures. This precursor is highly important for the understanding of the different film growth at low and high temperatures, which was investigated with high resolution low energy electron diffraction (HR- or SPA-LEED). Since the unit mesh of the commensurate monolayer is slightly different from the (102)-plane, considerable strain is accumulated during multilayer film growth. Nevertheless, at high substrate temperatures around 400 K, truly epitaxial films can be achieved without changes in the lateral geometric structure. On the contrary, films deposited at low substrate temperatures (< 160 K) relax towards the bulk structure already at a thickness of 3 ML. These results demonstrate that by an appropriate choice of the growth parameters, PTCDA films can deliberately be grown either in a strained epitaxial (i.e. substrate controlled) or a bulk like structure due to the existence of a precursor.

9:30 AM P9.4

GROWTH OF MULTICOMPONENT FILMS FROM ORGANO-METALLIC PRECURSORS: MONTE CARLO SIMULATIONS. Chaitanya Deo, University of Michigan, Dept. of Materials Science & Engineering, Ann Arbor, MI; David J. Srolovitz, Princeton University, Princeton Materials Institute & Dept. of Mechanical and Aerospace Engineering, Princeton, NJ.

Organometallic vapor phase epitaxy (OMVPE) is a leading technique for the deposition of multicomponent ceramic films. At present, quantitative relationships between OMVPE reactor conditions and film structure are poorly understood. In this presentation, we describe the development of a three-dimensional kinetic Monte Carlo (kMC) simulation method for OMVPE and apply it to the growth of two component $A_{0.5}B_{0.5}$ films. This simulation focuses on the surface reactions and does not include the reactive hydrodynamics within the gas phase. We employ model surface reactions representing decomposition of the precursors and etching of the surface species within the simulations. Growth on homoepitaxial, elemental and disordered substrates with {001} and {011} orientations is examined as a function of temperature and bond strength. The simulations are used to predict film structure, growth rates, surface roughness, terrace size, domain size, and the short range order parameter. The films are observed to grow relatively smoothly both by step growth and nucleation on terraces. The relative importance of these growth mechanisms varies with substrate and growth conditions. The films grow with roughnesses of order a single monolayer. Growth on elemental and disordered substrates leads to the formation of anti-phase boundaries (APBs). The growth rates are quantitatively related to the precursor decomposition kinetics. We will also present

preliminary results from the application of this kMC model to the OMVPE growth of the ferroelectric oxide $SrTiO_3$. A two-body central force interatomic potential is used to calculate bonding energetics and surface diffusion rate constants. Implications of these results for understanding OMVPE more generally are discussed.

10:00 AM *P9.5

CHARACTERIZATION OF SURFACE DEFECTS ON MgO THIN FILMS BY ULTRAVIOLET PHOTOELECTRON AND METASTABLE IMPACT ELECTRON SPECTROSCOPIES. A. Kolmakov, J. Stultz and D. Wayne Goodman, Department of Chemistry, Texas A&M University, College Station, TX.

Metastable impact electron spectroscopy (MIES) and ultraviolet photoelectron spectroscopy (UPS) have been used to investigate low-defective and defective MgO(100) thin films. Unlike low-defective films, defective films exhibit a new spectroscopic feature located at ~ 2 eV above the top of valence band. Exposing the defective film to oxygen quenches the emission of electrons from F-centers created on the surface and in the subsurface regions. Extended defects, unseen in the MIES spectra of the clean surface, are detectable using NO titration. MIES and thermal programmed desorption (TPD) indicate that at ~ 100 K NO adsorbs dissociatively on defects, forming N_2O . Only a small fraction of the MgO surface becomes covered with N_2O at ~ 100 K for the low-defective MgO film indicating that N_2O molecules preferentially adsorb on the extended defects. The saturation coverage of N_2O increases appreciably for the defective sample.

10:30 AM P9.6

THE HETEROEPITAXIAL NUCLEATION AND GROWTH OF METAL OXIDES BY IN SITU OXIDATION. Judith C. Yang, Guang Wen Zhou, Lori Tropa, Mridula Dixit Bharadwaj, Univ. of Pittsburgh, Dept of Materials Science and Eng., Pittsburgh, PA.

To gain unique insights into the fundamental oxygen-metal surface kinetics, we are investigating the initial stages of Cu thin film oxidation using in situ ultra-high vacuum (UHV) transmission electron microscopy (TEM). The advantages of in situ TEM experiments include visualization of oxidation processes in real time and information on buried interfaces. We have previously demonstrated that the initial stages of copper oxidation in dry oxygen is a surface-limited process, where oxide islands form epitaxially with the underlying substrate, even at atmospheric pressures. To quantitatively understand the nucleation to coalescence of the oxide film, we oxidized Cu(001) at 0.1 torr dry oxygen and 350C where the nucleation to coalescence can be clearly followed. We are presently modeling the nucleation to coalescence of the oxide film using the classical Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation and noted a qualitative agreement. We have examined the effect of different oxidizing atmospheres, such as water vapor, on the oxidation of metal surfaces.

10:45 AM *P9.7

MICROSTRUCTURAL AND SURFACE MORPHOLOGICAL EVOLUTION AT THE ATOMIC SCALE DURING THE GROWTH OF POLYCRYSTALLINE TiN: A HR-TEM, XRD, STM, AND MODELING STUDY. Joe Greene, S. Kodambaka, P. Desjardins, A. Vailionis, V. Petrova, I. Petrov, and D. Cahill, Materials Science Dept., Univ. Illinois, Urbana, IL.

XRD, TEM, and HR-XTEM analyses show that TiN grown by reactive evaporation or sputter deposition at low temperatures ($T < 450^\circ\text{C}$) exhibits competitive texture evolution with a columnar 111 kinetically-limited texture eventually becoming dominant. The columns are narrow and faceted with inter- and intracolumn porosity. Higher growth temperatures or the use of high incident N_2^+ /Ti flux ratios (> 5) with low N_2^+ energies (20 eV) result in non-competitive growth with a fully dense complete 002 orientation from the initial monolayer. The columns are broad-based with flat surfaces. Kinetic Monte Carlo modeling, assuming that the activation energy E_s for surface diffusion and the Ehrlich barrier E_b at descending step edges are larger on 111 than on 002, provide a qualitative understanding. Quantitative modeling requires transport activation energies (E_s , E_{edge} , E_f , and E_b) and island line tensions vs orientation. As a first step, we have grown single-crystal TiN(001) and TiN(111) layers at 700-950°C under conditions resulting in large ($> 1500 \text{ \AA}$) atomically-flat terraces. Partial TiN monolayers (0.1-0.4 ML) were then deposited and in-situ high-temperature STM used to following the coarsening and decay kinetics of single and multiple islands (Ostwald ripening) on flat terraces and in single-atom deep vacancy pits. From the results, combined with solutions of the Gibbs-Thompson and diffusion equations, we obtain the parameters listed above. The STM observations provide important atomic-scale insights into the growth of TiN and related transition-metal nitrides.

11:15 AM P9.8

LOW-DIMENSIONAL DEFECT-STRUCTURES OF NaCl(100) FILMS. Christoph Teegenkamp, Winfried Ernst and Herbert Pfnür, University of Hannover, Hannover, GERMANY.

We have investigated the morphology and the reactivity of epitaxially grown, stepped NaCl films on vicinal Ge(100) using LEED, UPS, EELS, and TDS. The generation of NaCl steps succeeds by using a 5.4° misoriented Ge(100) substrate towards the [011] direction. Supplementary, the amount of Ge steps with double atomic height, which is at least a necessary condition for the formation of NaCl steps with single atomic height, can be increased significantly by adsorption of 0.5 ML Si at 470 K.

In dependency of temperature, mainly two different NaCl growth modes of 8 ML thick films have been observed: Whereas NaCl molecules form at 300 K rectangular islands in [001] and [010] orientation, the NaCl film grows below 200 K layer-by-layer forming polar steps along the [011] direction. To characterize these step structures, in comparison to defect-free NaCl(100) and NaCl films covered with F-centres, both the band structure and the desorption behaviour of CO₂ has been investigated. The financial support by the Kali & Salz GmbH, Germany, and in addition by the University of Maryland/MRSEC, USA, is gratefully acknowledged.

11:30 AM P9.9

CONTROLLED NUCLEATION AND GROWTH OF NOBLE METALS ON POLYMERS. Vladimir Zaporozhchenko, Knut Behnke, Axel Thran, Thomas Strunskus, and Franz Faupel, Kiel Univ, Faculty of Engineering, Kiel, GERMANY.

In recent years research into the field of metal-polymer interfaces was mainly stimulated by applications of polymers in microelectronics packaging. Polymers are also seen as potential low-permittivity (low-k) dielectrics even for on-chip interconnects. Therefore, much effort has been made to understand and control the interfacial microstructure. The structure and properties of metal-polymer interfaces depends strongly on the deposition conditions and particularly the early deposition process plays a crucial role. Here the condensation coefficient *C* of noble metals on low-k dielectrics can be extremely low even at room temperature. The condensation and diffusion behavior of metal atoms in the initial deposition regime determines the nucleation and growth behaviour of the metal film. The weak interaction of noble metals with untreated polymers generally leads to Volmer-Weber type of growth with a critical nuclei consisting of only one metal atom. The nucleation probability and therefore the cluster density on the polymer surface can be varied over a wide range by a choice of the metal deposition conditions. Moreover, ion treatment of the polymer surface or the predeposition of a reactive metal also allows to vary the condensation coefficient and the cluster density in a controlled manner.

SESSION P10: METAL/SILICON AND GERMANIUM/SILICON EPITAXY
Chair: Joseph E. Greene
Thursday Afternoon, November 30, 2000
Room 302 (Hynes)

1:30 PM P10.1

CONDUCTIVITY AND MORPHOLOGY OF ULTRATHIN Pb FILMS ON Si(111) AT LOW TEMPERATURES. O. Pfennigstorf, A. Petkova, V. Borchers, J. Wollschläger and M. Henzler, Institut für Festkörperphysik, Universität Hannover, Hannover, GERMANY.

The electronic properties of thin metallic films strongly depend on its structure. For the preparation of ultrathin (0.8 ML up to 12 ML) and continuous films Pb was grown on a Si(111)-7×7-substrate at temperatures below 25 K. During growth or annealing a recrystallization of the films was observed by in situ SPA-LEED measurements. This effect also has a strong influence on the conductivity of the film. The disordered state of the thin films was observed up to a thickness of 4ML. Oscillations of conductivity during growth on annealed Pb layers point to nearly perfect layer-by-layer growth even at temperatures below 25 K. A direct comparison with the defect structure as measured in situ at low temperatures with SPA-LEED is possible for the classical size oscillations. A modulation of this oscillations shows an influence of the quantum size effect to the conductivity. The magnetoconductivity is strongly dependent on magnetic field due to superconducting fluctuations in two dimensional disordered and ordered superconductors. These fluctuations are reduced by surface roughness. These measurements show that magnetoconductivity of thin Pb films is dominated by superconductivity and weak localization up to 15 K. This temperature is far from the critical temperature of the bulk (7.2 K). The Hall voltage shows an oscillating sign for the films from 0.8 up to 12 ML thickness. Here quantum size effect is seen both for disordered (up to 4 ML) and ordered films.

Therefore the combination of measurements of films with different thickness and morphology and at different temperature and magnetic field enables the separation of different scattering mechanisms including the scattering times.

1:45 PM P10.2

A HIGH-TEMPERATURE STM-STUDY OF IRON SILICIDE FORMATION ON HIGH INDEX SILICON SURFACES. Volker Dorna, Martin Knepppe, Evgueni Kot, Ulrich Köhler, Ruhr-Universität Bochum, Bochum, GERMANY.

The nucleation and initial growth of iron silicide on Si(1 1 3), Si(5 5 12) and Si(1 1 4) is studied in comparison to Si(111) using high temperature STM. During MBE and gas source deposition (precursor Fe(CO)₅) STM-“movies” at temperatures up to 600°C directly show the kinetics of the alloy formation on the surface. Whereas on Si(111) 3D-silicide islands already form in the sub-monolayer range, a complete wetting layer is formed on all vicinal surfaces for temperatures below 560°C. A mixture of different periodicities (4xn), with *n* ranging from 2-6, is found. The closed wetting layer strongly hinders the vertical outdiffusion of silicon and for gas source deposition further growth is slowed down dramatically. Above 1 ML, growth proceeds with strongly anisotropic 3D-silicide islands with aspect ratios up to 50. Especially on Si(1 1 4) this way a perfectly one-dimensional nanostructured silicide layer can be grown. A lateral spreading of the 3D-islands can be achieved by a stoichiometric co-deposition of Fe and Si. On Si(5 5 12) prolonged annealing of the iron covered silicon surfaces leads a complete faceting of the substrate with a mixture of silicide areas and completely clean areas.

2:00 PM P10.3

COHERENT X-RAY DIFFRACTION FROM MICRON SIZED GOLD CRYSTALS. M.A. Pfeifer, G.J. Williams, I.K. Robinson, Univ of Illinois, Dept of Physics, Urbana, IL.

As evaporated on inert SiO₂ substrates, Au films are polycrystalline with {111} texture. High temperature annealing causes dewetting and eventually crystallization into micron sized particles. The diffraction pattern from a coherently illuminated object is simply the Fourier transform of the object. Because in an X-ray experiment it is only possible to record the amplitude and not the relative phases of the diffracted waves, the diffraction pattern cannot be uniquely inverted. However, through iterative techniques it is possible to recover the lost phase and, hence, the shape of the diffracting crystal. It is with this in mind that we collected 3D diffraction patterns from near-equilibrium Au crystallites. We measured Au crystallites with a size of 0.5 to 2 microns using a 10 keV X-ray beam at Sector 33 of the Advanced Photon Source, Argonne National Laboratory. 2D slices through the diffraction pattern were obtained with a CCD camera. 3D information was gathered by taking images at different diffractometer angles. Strong streaks appear perpendicular to the facets presented; these were modulated into fringes when pairs of facets occurred.

2:15 PM P10.4

NUCLEATION AND COARSENING EVENTS IN POLYCRYSTALLINE THIN FILMS OBSERVED BY *IN SITU* TRANSMISSION ELECTRON MICROSCOPY. F.M. Ross, R.M. Tromp, IBM Research Division, T.J. Watson Research Center, Yorktown Heights, NY; and D.N. Dunn and R. Hull, Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA.

In situ transmission electron microscopy techniques have been extremely valuable in clarifying growth mechanisms in epitaxial films, allowing us to measure, for example, the kinetics of self-assembled island formation and the dynamics of dislocation motion as strained films relax. We have applied similar in situ microscopy techniques to the study of nucleation and growth in polycrystalline thin films. Polycrystalline films present us with the opportunity to observe phenomena not possible in epitaxial films, such as nucleation and coarsening events in grains of different orientation and the development of texture. Metals such as Ti or Al are evaporated under UHV onto an electron transparent substrate in the microscope polepiece while simultaneously acquiring images or diffraction patterns at video rate. The texture and grain structure are observed continuously as the film grows, and the UHV environment allows us to characterize reactive materials such as Ti without atmospheric contamination. In the case of Ti films deposited onto oxidized silicon substrates we observe a change in texture from [hk0] to [001] as the film grows thicker than 2.5nm; we attribute this to changes in surface energy associated with the known diffusion of oxygen from the substrate into the first 1-2nm of the film. By recording grain coalescence events we can measure parameters such as surface diffusion coefficients. We will present these results and we will also discuss experiments aimed at characterizing grain nucleation and coarsening in polycrystalline copper. In these experiments the copper film is deposited electrochemically in situ using a novel design of wet

cell, including electrical contacts and an electrolyte reservoir, which is compatible with the microscope environment.

2:30 PM P10.5

KINETIC AND STRAIN-INDUCED GROWTH INSTABILITIES OF $\text{Si}_{1-x}\text{Ge}_x$ EPI-LAYERS ON VICINAL $\text{Si}(001)$. Christoph Schelling, Gunther Springholz, Friedrich Schäffler, Institut für Halbleiterphysik, Universität Linz, Linz, AUSTRIA; Markus Sulzberger, Bert Voigtländer, Institut für Grenzflächenforschung, FZ Jülich, GERMANY.

Compressive in-plane strain was considered to initiate roughening of pseudomorphic SiGe heterolayers through a bunching of steps. Recently, we found (cf. Ref. 1) that under growth conditions far from thermal equilibrium Si homoepitaxial layers develop kinetically driven surface corrugations of similar appearance. Since device applications require flat interfaces, it is important to discriminate kinetic and strain-induced growth phenomena. Here, STM measurements of Si buffers will be presented, which provide new insights into the kinetic mechanisms of Si homoepitaxial growth. Tuning the growth conditions, it is possible to fabricate Si buffers that are either atomically flat or provide a kinetically roughened template with adjustable amplitude and period. On this base we systematically studied the morphology of strained $\text{Si}_{1-x}\text{Ge}_x$ layers deposited either under kinetically limited, or under equilibrium growth conditions. By increasing the composition from $x=0.05$ to $x=0.5$ the compressive in-plane strain was varied between 0.2% and 2.1%. With atomically flat buffers, and for substrate miscuts between 0.05 and 4.3° we found no indications for strain-driven one-dimensional step bunching. Instead, we observe elongated hut-clusters under kinetically limited growth conditions that evolve into square based pyramids near thermal equilibrium. On the other hand, low-composition SiGe layers grown on corrugated Si buffers basically replicate the buffer morphology. It is most likely this phenomenon that has led to the erroneous reports on strain-induced one-dimensional step-bunching in the literature. [1] C. Schelling et al., Phys. Rev. Lett. 83, 995 (1999)

2:45 PM P10.6

LATERAL SELF ORGANIZATION OF Si QUANTUM DOTS BY PERIODIC SUBSURFACE DISLOCATIONS ARRAYS. Franck Fournel, Karine Rousseau, Joel Eymery, Jean Luc Rouviere, Denis Buttard, Noel Magnea, CEA-Grenoble, Dept. de Recherche Fondamentale; Hubert Moriceau, Bernard Aspar, CEA-Grenoble, LETI/Dept. Microtechnologie; Thierry Baron, INSA-Lyon, Lab. Phys. de la Matière; Pierre Mur, Francois Martin, Marie Noelle Semeria, CEA-Grenoble, LETI/Dept. Microelectronique, Grenoble, FRANCE.

The lateral self-organization of Si dots by a buried array of subsurface dislocations is evaluated on 4 inches (001) bonded silicon wafers. The buried dislocation superlattice is obtained by transferring a 10 nm thick silicon film on commercial (001) Si wafers by using the combination of SOI technologies and hydrophobic bonding. The values of the precisely controlled twist and tilt angles between the film and the substrate define the period of the surface strain field created by the screw and the edge dislocation networks. A combination of grazing incidence X-ray diffraction, TEM and STM measurements confirm that only the elastic strain field propagates up to the surface and produces a nanoscale patterning of the bonded film surface which will control the nucleation process. STM images shows that self assembled nanocrystals deposited on such templates form an ordered array of quantum size nanostructures. These experimental data show that the random nucleation has been suppressed and that the 2D periodicity of the dislocation network has been transmitted to the islands superlattice. This result can be interpreted in the framework of the recent theoretical proposals of A.E. Romanov et al. -APL 74, 2280,1999-and A. Bourret -Surface Science 432, 37, 1999- that analyse the influence of buried stressors on surface energy. This technique of lateral organization should have all the requirements for a large scale integration of ordered nanostructures in term of size, dispersion and density.

3:30 PM P10.7

NON-LINEAR GRINFELD INSTABILITY OBSERVED IN MULTILAYER $\text{Ge}/\text{Si}(100)$ STRUCTURES. Woei Wu (Larry) Pai, H.H. Cheng, Center for Condensed Matter Sciences, National Taiwan University, Taipei, TAIWAN.

A surface under uniaxial stress is morphologically unstable with respect to mass rearrangement. The destabilizing force is of elastic origin and is countered by surface tension that prevents short wavelength deformation. This is the so-called Grinfeld instability. Non-linear analysis indicates trench formation, and it has been surmised that fracture and 'coherent' Stranski-Krastanov growth are related to this instability. Since recent developments of semiconductor heteroepitaxy often call for sophisticated control of surface and interface morphology, it is increasingly recognized that a deeper understanding of Grinfeld instability is critical. We therefore prepared

a series of samples by molecular beam epitaxy in which six bi-layers of $\text{Ge}/\text{Si}(100)$ ($\sim 1\text{nm}/30\text{nm}$) were grown at 260C and 450C respectively. The uncapped samples were terminated at Ge layers. We found the surface morphology is extremely sensitive to the Ge coverage. Within a range of ± 0.2 nm and with an increasing Ge thickness, the surface evolves from states of (1) slight undulation, (2) deep trenches, to (3) flatness, as measured by ex situ ambient AFM. Surprisingly, the depths of trenches in (2) extend to over $\sim 20\text{nm}$. That is, they penetrate deep into the Si spacer. This contradicts the general thought that trench growth should be effectively limited as it approaches substrate or interface because the local stress field at the trench tip reverses sign. Furthermore, the $\sim 300\text{nm}$ wavelength of the trench pattern is unexpectedly long. Cross sectional TEM was also used to corroborate the structure information obtained by AFM. We found sample (1) was mostly elastically strained with few misfit dislocations. Sample (2) was similar to (1) except that we observed formation of novel vertically collimated 'inverted dots' beneath the Ge layers. Sample (3) was heavily relaxed due to misfit dislocations. This suggests the non-linear Grinfeld instability as the precursor for misfit dislocation nucleation. The dependence of the observed instability on temperature and different layer structures will also be discussed.

3:45 PM P10.8

SURFACE MORPHOLOGY OF SiGe EPITAXIAL LAYERS GROWN ON UNIQUELY ORIENTED Si SUBSTRATES. Morgan Ware and Robert Nemanich, North Carolina State University, Physics Dept, Raleigh, NC.

The 4% lattice mismatch between Si and Ge creates strain in epitaxial layers of SiGe alloys on Si, and this strain can manifest itself in the morphological structure of the surface of the epitaxial layer. This study explores the relationship of the evolution of the surface morphology of SiGe layers grown on a range of Si surface orientations. We have grown layers of $\text{Si}(0.7)\text{Ge}(0.3)$ to 100nm by solid source MBE on substrates with surface normals rotated from [001] to [111] by angles of $\theta = (0, 2, 4, 10, 22)$ degrees. The surface morphology was investigated by atomic force microscopy, which showed considerable ordering of surface features. These features evolve from hut-like structures at 0 degrees to large mesa-like structures separated by pits and ridges at 22 degrees. The organization of these features is also shown to vary with the substrate orientation. Each surface has characteristic lines along which features are aligned, and these lines vary continuously with the angle of rotation of the substrate. The state of relaxation of each layer is quantified by Raman spectroscopy so that a direct correlation between residual strain and surface morphology can be made.

4:00 PM P10.9

DIRECT OBSERVATION OF ELECTROMIGRATION OF SILICON MAGIC CLUSTERS ON $\text{Si}(111)$ SURFACES. Ing-Shouh Hwang, Mon-Shu Ho, Tien T. Tsong, Institute of Physics, Academia Sinica, Nankang, Taipei, TAIWAN ROC.

A special type of Si magic clusters on $\text{Si}(111)$ surfaces are found with a variable-temperature scanning tunneling microscope (STM). They play an important role in mass transport phenomena, step fluctuations, and epitaxial growth. We characterize the structure of these clusters and derive path-specific hopping parameters using Arrhenius analysis [1]. Interestingly, when a Si magic cluster hops out of a 7×7 half-cell, it usually reappears at a site a few hundred Å away. The most interesting behavior seen in the long hops of Si magic clusters is that the clusters have a bias (65-80%) for motion in the direction toward the cathode. Effects of the directed motion along the direction of the heating current in electromigration and those in thermal migration are determined separately and quantitatively. We also observe the preferential presence of Si magic clusters at the corner of Si craters near the cathode side and their subsequent attachment to that corner as well as the preferential detachment of Si magic clusters from Si bilayer island edges near the cathode side. As the electric fields we apply (on the order of 1-10 V/cm) are very small, the strong tendency for these biased phenomena is very surprising [2]. [1] I.-S. Hwang, M.-S. Ho, and T.T. Tsong, PRL 83, 120 (1999). [2] M.-S. Ho, I.-S. Hwang, and T.T. Tsong, to appear in the June 19 issue of PRL 84 (2000).

4:15 PM P10.10

NUCLEATION AND GROWTH KINETICS OF DIMER-ADATOM-STACKING-FAULT STRUCTURES ON LASER-ETCHED $\text{Si}(111)$ SURFACES. Kazuyoshi Shimada¹, Tetsuya Ishimaru^{1,2}, Takanobu Watanabe¹, Takuya Yamawaki¹, Mariko Osuka¹, Tadatsugu Hoshino³ and Iwao Ohdomari^{1,2}. ¹School of Science and Engineering, Waseda University, Tokyo, JAPAN; ²Kagami Memorial Laboratory for Materials Science and Technology, Waseda University, Tokyo, JAPAN; ³Faculty of Pharmaceutical Sciences, Chiba University, Chiba, JAPAN.

Investigation of Si surface reconstruction is important, not only for

physical interest but also as a guiding principle for nanostructure fabrication. In this work, nucleation and growth kinetics of dimer-adatom-stacking-fault (DAS) reconstruction on Si(111) surfaces have been investigated by measuring the time evolution of DAS domain size distribution at four temperatures ranging 360-440°C. The experiments were performed using a scanning tunneling microscope (STM). The 7x7 DAS structures spreading over the whole surface maintained at high temperature were destructed by a nano-second-pulsed laser irradiation. After keeping the specimen at growth temperature, the surface was quenched to room temperature and numerous STM images were obtained in order to extract the size distribution of DAS domain. The experimental results clearly show that the higher the substrate temperature is, the faster the DAS domain grows. The whole feature of the growth is similar at every growth temperature, which reveals the following two different kinetics of the reconstruction. At the very early stage, the surface contains many voids induced by laser irradiation and the DAS reconstruction is quite rapid. The density of the voids is in the same order as that of the DAS domains formed initially, which suggests that the DAS reconstruction is promoted around the voids. At the next stage, after the disappearance of the voids, the DAS domains develop in a measurable time scale. Based on the two-dimensional nucleation and growth theory, we have performed fitting calculations for the domain size distributions and have found that the DAS domains nucleate and grow steadily at each temperature. The activation energies for the formation and the annihilation of the DAS structure have been estimated to be 1.6 ± 0.4 and 2.1 ± 0.6 eV, respectively. The difference in the two activation energies reflects the stabilization of DAS domain upon growth.

4:30 PM P10.11

A GROWTH TECHNIQUE FOR PRODUCING EXTENSIVE ATOMICALLY FLAT SURFACES ON SILICON. Dooan Lee, Todd Schroeder, James Engstrom and Jack Blakely, Cornell Center for Materials Research, Ithaca, NY.

We have been successful in producing arrays of mesas on Si(111) which are free from atomic steps. These are of interest in CMOS technology and for quantum well structures. They also provide interesting substrates for fundamental surface science experiments. In previous work we have created atomically flat regions surrounded by ridges through an evaporation method. The present work 'inverts' the previous process by using a pattern of trenches to define the mesas and then depositing Si to grow the atomic steps off the edges. The mesas are created on Si wafers, which are $\sim 0.3^\circ$ from the (111) plane by lithography and reactive ion etching. Both the evaporation and this new growth technique rely on step flow to move the steps to the edges of the flat areas. Although the evaporation method is simpler, an advantage of the growth technique is that it can be carried out at lower temperature. The maximum size of mesa that can be made free of atomic steps depends on the combination of temperature and deposition rate. On very large step-free terraces nucleation of islands and concentric arrays of mono-atomic steps are observed; these correspond to the vacancy pits observed with the evaporation method.

4:45 PM P10.12

IN SITU OBSERVATION OF INSTABILITY IN STEP MORPHOLOGY DURING EPITAXY AND EROSION. P. Finnie^a and Y. Homma, NTT Basic Research Laboratories, Atsugi, JAPAN. ^aNew address: National Research Council, Ottawa, CANADA.

Instability in the morphology of atomic steps is expected for certain growth conditions [1]. To test and extend this prediction, various atomic step geometries were prepared on ultra-flat Si(111) substrates. Atomic steps were observed using an in situ scanning electron microscope. For specific growth conditions and certain step arrangements unstable growth was observed [2]. While the growth was stable at low fluxes, at higher fluxes the step shape became irregular, and even dendritic. The same instability also causes wandering step profiles which are often seen after sublimation, but were previously poorly understood [3]. For both growth and sublimation, terrace widths play an essential role in the instability. Given the observed crystalline symmetry of the step velocity in the unstable regime, some elaboration to the elementary theory is required. [1] G.S. Bales and A. Zangwill, Phys. Rev. B 41 (1990) 5500 [2] P. Finnie and Y. Homma, Phys. Rev. Lett., to be published [3] Y. Homma and P. Finnie, J. Vac. Sci. A, to be published

SESSION P11: POSTER SESSION
METAL ON SEMICONDUCTOR AND
SEMICONDUCTOR THIN FILMS
Chair: John F. Wendelken
Thursday Evening, November 30, 2000
8:00 PM
Exhibition Hall D (Hynes)

P11.1

RELATIONSHIP BETWEEN GRADED LAYER STRUCTURES AND DEFECTS IN SILICON-GERMANIUM VIRTUAL SUBSTRATES. Kazuki Mizushima, Ichiro Shiono, Kenji Yamaguchi, Mitsubishi Materials Corporation, Central Research Institute, Omiya, JAPAN; Naoki Muraki, Mitsubishi Materials Silicon Corporation, Noda, JAPAN.

A silicon-germanium virtual substrate provides desirable way to fabricate a strained-silicon field-effect transistor. However high threading dislocation density and rough surface morphology limit the capability of the substrate. In order to reduce the defects, we investigated relationship between graded layer structures and defects in the virtual substrates. The virtual substrates were synthesized by low-pressure chemical vapour deposition (LPCVD) by using SiH₄, GeH₄, and carrier H₂ gases. A graded Ge composition layer (graded layer) followed by a constant Ge composition layer (buffer layer) was deposited on a Si(001) substrate. The typical Ge composition was zero to 30% in the graded layer and 30% in the buffer layer. Typically the grading rate in the graded layer and the thickness of the buffer layer were 20%/μm and 0.75μm, respectively. To vary the Ge profile in the graded layer we considered linear-graded structures, rectangular-step structures, and graded-step structures. We measured threading dislocation density at the surface region by Secco etching. The surface roughness was measured by Nomarski type scanning instrument and atomic force microscopy (AFM). Also we observed the dislocations in the samples by transmission electron microscopy (TEM). We found both of the threading dislocation density and the surface roughness were reduced in the graded-step structures compared to that of the linear-graded structures. Also there was an optimized number of steps which showed minimum dislocation density and surface roughness. On the other hand we found that, in the rectangular-step structures, the threading dislocation density increased as number of step was increased, although surface roughness was reduced. We consider the Modified Frank-Read mechanism to understand the results in conjunction with the TEM observations.

P11.2

STRAIN-INDUCED DIFFUSION IN STRAINED SiGe/Si HETEROSTRUCTURES. Young Soo Lim, Dept. Materials Sci. & Eng., KAIST, Taejeon, KOREA; Jeong Yong Lee, Dept. Materials Sci. & Eng., KAIST, Taejeon, KOREA; Hong Seung Kim, SiGe Device Team, ETRI, Taejeon, KOREA; Dae Won Moon, Surface Analysis Group, KRISS, Taejeon, KOREA.

Diffusivity in a strained heterostructure was theoretically investigated, and general diffusion equations with strain potential were deduced. There was an additional diffusivity by strain potential gradient as well as by the concentration gradient. The strain-induced diffusivity was a function of Ge concentration, and its temperature dependency was formulated. The activation energy of the strain-induced diffusivity was measured by high-resolution transmission electron microscopy in a SiGe/Si heterostructure. This result can be generally applied for the investigation of the diffusion in strained heterostructures.

P11.3

AB INITIO STUDY OF Ge ADSORPTION ON H-TERMINATED Si(001) SURFACES. Takahisa Ohno, Jun Nara, Natl Res Inst for Metals, Tsukuba, JAPAN.

We have theoretically investigated adsorption and diffusion of Ge atoms on the monohydride terminated Si(001) surface by using first-principles total-energy calculations, in order to unveil the surfactant effects of hydrogen atoms on the Ge/Si heteroepitaxial growth. The Ge atom deposited on the H/Si(001) surface exhibits a number of metastable geometries in the form of either monohydride or dihydride. There are two types of diffusion processes, which have different activation energies. At lower temperatures, the Ge adatom diffuses along the Si dimer rows by repeating site exchange with substrate Si atoms, which has an activation barrier of as small as 0.75 eV. At higher temperatures, the most stable geometry for the deposited Ge atom is thermally realized, which has a substrate Ge-Si dimer and a Si adatom having a dihydride structure, as a result of the site exchange. The Si adatom can diffuse away from the substrate Ge-Si dimer, while the substrate Ge atom can also diffuse as an adatom after it exchanges sites with the Si adatom again. In this way, Si atoms as well as Ge atoms become diffusing species at higher temperatures. The activation energies of these diffusion processes are about 1.30 eV, which are extremely larger than that on the bare Si(001) surface. The reduction of the surface diffusion results in the increase in the number of nucleation centers, which may explain the growth mode change from islanding to layer-by-layer growth. As a result of two types of diffusing species, that is, Ge and Si, the ad-dimers formed in the initial stage of the Ge growth on the H/Si(001) surface is supposed to be not only Ge-Ge dimers but also Ge-Si and Si-Si dimers. This effect will be conspicuous at low growth rates and high temperatures.

P11.4

STM STUDY OF NUCLEATION PROCESSES DURING ION-ASSISTED MBE GROWTH OF Ge ON Si SURFACES.

Jiro Matsuo, Toshio Seki, Gikan H. Takaoka, Ion Beam Engineering Experimental Laboratory, Kyoto University, Kyoto, JAPAN; Isao Yamada, Laboratory of Advanced Science and Technology for Industry, Himeji Institute of Technology, CAST, Ako, JAPAN.

Ion assisted technique is widely used for high quality film formation. However, the role of ion bombardment during film formation is not well understood. Ion bombardment effects on surfaces and nucleation growth at various temperatures have been studied with the Ultra High Vacuum Scanning Tunneling Microscope (UHV-STM). In order to reveal the role of ion bombardment during film formation, ion bombardment effects at the each stage of film formation have been investigated. The single ion impact traces whose diameters were about 20 Å were clearly observed with atomic resolution on the Si(111) 7×7 surface irradiated with Xe ions. After annealing at 400°C, the vacancies created in subsurface by the impact start to diffuse toward the surface and appear on the surface. At 600°C, the vacancy clusters whose sizes correspond to the number of the vacancies created near the surfaces are formed. These vacancy clusters play a very important role in Ge films growth. After annealing of a Si(111) sample at 400°C with Ge atoms deposited to a few Å, many Ge islands was observed on the surface. These islands did not separate nor coalesce into step edges when the surface with the Ge islands was irradiated by Xe ions at dose of below 10¹⁴ ions/cm². Number of vacancies is less than the number of Ge atoms. When the ion dose was above 10¹⁴ ions/cm², Ge islands disappeared, and the surface morphology was completely changed. Growth kinetics modified with ion irradiation will be discussed.

P11.5

POLYCRYSTALLINE Si_{1-x}Ge_x LAYER GROWN BY THE UHV-CVD AND UHV-ECRCVD. Jin-Won Park, Hwan-Kuk Yuh, Seung-Hyun Lim, Hong-Ro Lee, Euijoon Yoon, School of MS&E, Seoul National University, Seoul, KOREA; Jong-Ho Lee, Electrical Engineering, Wonkwang University, Iksan, KOREA.

Polycrystalline Si_{1-x}Ge_x film is a promising alternative to a conventional polycrystalline Si film gate material in CMOS devices due to its ease of lower temperature growth, higher dopant activation rate, less gate depletion effect and less boron penetration. In this study, we investigated the growth characteristics of polycrystalline Si_{1-x}Ge_x films by ultrahigh vacuum chemical vapor deposition (UHV-CVD) and ultrahigh vacuum electron cyclotron resonance chemical vapor deposition (UHV-ECRCVD). Polycrystalline Si_{1-x}Ge_x films deposited on oxidized wafers using SiH₄ and GeH₄ in the temperature ranges of 400 - 700°C. Thin film characteristics were studied by SEM, TEM, RBS, XRD, and AFM. As the growth temperature increased, the growth rate of SiGe films increased. However, at temperatures above 650°C, film growth was severely inhibited, especially when Ge content was above 40%. Effects of pretreatment of the silicon oxide surface by GeH₄ was also studied. Without the GeH₄ pretreatment, three-dimensional islands were grown at 550°C, leading to discontinuous films with a rough surface. On the other hand, 2-min GeH₄ pretreatment made the polycrystalline Si_{1-x}Ge_x layer continuous and smooth at the same growth conditions. It is speculated that the GeO was desorbed from the oxide surface during the pretreatment, consequently the surface became Si-rich, providing easy nucleation sites on the oxide surface. This new growth technique may help us overcome the difficulty of polycrystalline Si_{1-x}Ge_x layer deposition on oxide. We will also discuss the changes in film morphology and microstructures with surface chemistry of the oxide film. Differences in growth mechanism between UHV-CVD and UHV-ECRCVD will be also addressed.

P11.6

STRUCTURAL QUALITY OF VIRTUAL SUBSTRATES AND Ge-RICH CHANNELS FOR HIGH-SPEED SiGe p-MOS DEVICES.

Matthias Kummer, Hans von Känel, Laboratorium für Festkörperphysik, ETHZ, Zürich, SWITZERLAND.

Fully relaxed, linearly graded Si_{1-x}Ge_x buffer layers with x between 0.5 and 0.7 serve as virtual substrates for thin, coherent Ge-rich channels (up to pure Ge), for p-MOS devices with high hole mobilities [1]. The films for this study have been grown with low energy plasma enhanced chemical vapour deposition (LEPECVD), at temperatures of 600-720°C, using growth rates between 3 and 5 nm/s. The typical layer thickness was between 5 and 8 μm. High resolution x-ray diffraction was used to investigate the degree of relaxation and the overall structural quality of the films. The surface morphology was measured using atomic force microscopy (AFM). Thin compressively strained channels with high Ge concentrations have been deposited on top of the virtual substrates at temperatures below 500°C and using lower plasma densities in order to suppress strain-induced surface

buckling. [1] G. Höck, E. Kohn, C. Rosenblad, H. von Känel, H.-J. Herzog, and U. König, Appl. Phys. Lett. (in press)

P11.7

Ge SEGREGATION IN THICK STRAINED SiGe/Si(001) FILMS GROWN AT HIGH RATES. Matthias Kummer, Hans von Känel, Laboratorium für Festkörperphysik, ETHZ, Zürich, SWITZERLAND; Enver Kh. Mukhamedzhanov, Shubnikov's Institute of Crystallography, Moscow, RUSSIA; Alex Dommann, Institut für Mikrosystemtechnik, NTB, Buchs, SWITZERLAND.

Strained epitaxial Si_{1-x}Ge_x films with shallow, linear Ge composition profiles have been grown by low energy plasma enhanced chemical vapour deposition (LEPECVD) at temperatures between 600°C and 700°C. The films were grown to thicknesses between 5 μm and 20 μm, with final Ge concentrations between 2% and 0.5%. High resolution x-ray diffraction (HRXRD) has been employed to investigate the actual composition and structural quality of the films. It turned out that despite of growth rates between 2.8 and 5.7 nm/s, and the low Ge concentrations, significant Ge segregation takes place, leading to a Ge enriched surface layer several hundred nm in thickness, with top Ge concentrations of up to 5-10 times the nominal maximum value. The segregation can efficiently be suppressed using additional H₂ acting as a surfactant during growth.

P11.8

RAMAN SPECTROSCOPIC STUDY OF STRESS AND DISORDER IN SURFACTANT-MEDIATED MBE GROWN Ge(211)/Si(211).

G. Brill, S. Tari, S. Sivananthan, Univ of Illinois at Chicago, Physics Dept, Chicago, IL; Y. Gogotsi, Univ of Illinois at Chicago, Dept of Mechanical Engineering, Chicago, IL.

Ge grows on Si in the Stranski-Krastanov growth mode (2D-3D) because of the 4.2 % lattice mismatch between materials. However, this growth mode can be altered to the Frank-Van der Merwe (layer-by-layer) growth mode by depositing a suitable surfactant prior to nucleation of the Ge layer. By utilizing surfactant-mediated growth in the (001) and (111) orientations, island-free nucleation of Ge can be obtained up to thicknesses that are many times greater than the critical thickness for Ge nucleated directly onto Si without a surfactant. Moreover, the surfactant acts to suppress Ge-Si alloy formation at the substrate interface. In this study, we have nucleated thin Ge layers on Si(211) substrates with and without As deposition before Ge growth to study the effect of surfactant-mediated growth in the (211) orientation. The layers were monitored in-situ by reflection high-energy electron diffraction (RHEED) and were characterized ex-situ by Raman spectroscopy. Initial results confirm that the growth mode is altered significantly by saturating the Si surface with a monolayer of As prior to Ge growth. Measurements of peak shifts and peak widths in the Raman spectra show that more disorder and alloying are present for layers grown without the surfactant. However, alloy formation is not completely suppressed for layers nucleated with the aid of a surfactant, contrary to Ge grown on Si in the (001) orientation. These results as well as a simple growth model will be presented describing the differences between surfactant mediated growth in the (211) and (001) orientations.

P11.9

OPTICAL PROPERTIES OF SELF-ORGANISED SSMBE AND GYMBE Ge NANOSTRUCTURES GROWN ON SiGe TEMPLATE LAYERS ON Si (118). G. Bremond, P. Ferrandis, A. Souifi, INSA de Lyon Laboratoire de Physique de la Matière, UMR 5511CNRS, Villeurbanne, FRANCE; M. Abdallah, A. Ronda, I. Berbezier, CNRS, Centre de Recherche sur les Mécanismes de la Croissance Cristalline, Marseille, FRANCE.

The control of Ge/Si self-organized low dimensional nanostructures becomes very important due to the great potentiality of this semiconductor system for theoretical and technological application in nanoelectronics and optoelectronics. This work reports on the photoluminescence properties of single quantum well and multiple quantum wells consisting in double layer structures (Ge(n)/Si_{1-x}Ge_x) deposited on Si substrates realised by gas source MBE (GS-MBE) and solid source MBE (SS-MBE). The process used consists in realising in a first step a Si_{1-x}Ge_x template layer with a "self-patterned" morphology. Such patterning, based on periodic morphological modulation of the surface is used to confine and organise the Ge dots in a second deposition step. Between the two deposition steps, a short annealing is performed to allow the equilibrium Ge segregation and limit further Si/Ge interdiffusion during Ge dots deposition on the template layer. The PL providing from the 2D wetting layer in the case of $n = 3$ ML has been found to be more intense in GS-MBE thanks to the passivating rule of the hydrogen atoms. The 2D to 3D growth transition is accompanied by the occurrence of a red-shifted large PL band (L) attributed to dots. While broadened red-emission is obtained from dots directly deposited on Si substrate, narrower band is obtained from dots deposited on the template layer. Moreover

the red-shift of the (L) band observed in the latter case is attributed to higher Ge concentration in the dots. In the other hand, there is no effect of the hydrogen on the formation of the islands which show similar optical and structural properties in the both growth techniques. The main difference between GS-MBE and SS-MBE concerns a low energy shift in the PL of the SSMBE Ge dots that we shall discuss the interpretation due to size, dispersion and Ge concentration or strain effects.

P11.10

GROWTH CHARACTERISTICS OF Si AND SiGe ON DIFFERENT PATTERN DENSITIES DURING A SELECTIVE EPITAXIAL GROWTH. Sukchan Song, Euijoon Yoon, Seoul National Univ, School of Materials Science and Engineering, Seoul, KOREA; Soo-Min Lee, Seu-Ho Lee, ASB, Inc., Taejon, KOREA; Young-Ho Lee, Soo-Kyun Park, Daewoo Electronics Co., Ltd., Seoul, KOREA.

SiGe selective epitaxial growth (SEG) technology has been widely studied to form a thin base layer in heterojunction bipolar transistors (HBTs). No deposition is expected on dielectric mask areas to be incorporated successfully in the device fabrication. However, changes in surface chemistry of the dielectric mask materials sometime lead to nodule formation on the mask area. Also, any possible changes in adatom diffusion characteristics would affect the SEG characteristics. In this report, we present the characteristics of Si and SiGe selective epitaxial growth on Si (001) wafers with different oxide pattern densities. Growth was made in a commercial RPCVD system with H₂, SiH₂Cl₂, GeH₄, and HCl gas-mixtures as source gases. The growth temperature varied from 750 to 775°C and a pressure was fixed at 40 Torr. Scanning electron microscopy (SEM) and Nomarski interference microscope were used to analyze selective growth characteristics. We found that the nucleation behavior of the Si and SiGe on the oxide was quite distinct from each other. The SiGe nodule (i.e., nucleus) distribution varied with different oxide pattern densities, whereas that of Si nodules was independent of oxide-pattern density. In addition, SiGe nodule density decreased as the oxide pattern density increased. In the case of SiGe SEG, the surface composition would be Si-rich with GeH₄ exposure by forming volatile GeO. However, changes in pattern density would vary the effective Ge adatom concentration and change the surface chemistry of the oxide surface, consequently the SiGe nodule density. Detailed mechanism will be discussed.

P11.11

THERMODYNAMICS OF C ENRICHED Si(100) FROM AB INITIO CALCULATIONS. I.N. Remedakis^{1,2}, Efthimios Kaxiras¹ and P.C. Kelires². ¹Department of Physics and Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA; ²Physics Department, University of Crete, Heraclion, Crete, GREECE.

The adsorption of C on the Si(100) surface is a challenging problem for both applied and basic research. It is a representative example model for the surface of group-IV semiconductor alloys, which are of great importance in technology. For instance, a high speed transistor based on B-doped SiGeC alloy has been very recently manufactured. The differences and similarities in the two components, Si and C, together with the nature of the Si(100) surface, give rise to several interesting phenomena: C incorporates into the Si lattice because of the enhanced surface mobility, despite that its bulk equilibrium solubility is of the order of 10⁻⁹; the surface reconstruction changes from (2 × 1) or (2 × 2) to a c(4 × 4) periodicity; in contradiction to the empirical rule that the most electronegative atoms prefer to be located at surface sites, C seems to prefer subsurface sites. The atomistic features of these systems are not clear at present. In this study, we approach the problem of C incorporation in the Si lattice from a thermodynamic perspective. The procedure we follow has two steps: Firstly, we perform *ab initio* electronic structure calculations, considering every possible configuration for the system under study to obtain the few lowest energy structures. Secondly, we construct a classical effective Hamiltonian, with its parameters determined from the atomistic calculations. Using this Hamiltonian in a Monte Carlo scheme, we are able to study the thermodynamic properties, taking into account both the temperature and the C composition during the deposition process, the latter entering into the model through the chemical potential difference between C and Si. Our study elucidates a number of experimental observation of this intriguing system.

P11.12

MORPHOLOGICAL INSTABILITIES DURING EXPLOSIVE CRYSTALLIZATION OF GERMANIUM FILMS. Aleksandra Chojnacka, Michael Thompson, Cornell Univ, Dept of Materials Science and Engineering, Ithaca, NY.

Explosive crystallization of germanium exhibits three distinct kinetic and morphological regimes. Dynamics of the growth processes, and the resulting morphologies, have been examined in detail. Analyses of the experimental and computational results provide evidence for two distinct processes governing the explosive

crystallization in the high and low temperature limiting regimes. Steady-state crystallization velocities were measured as a function of substrate temperature, which controlled heat loss into the substrate. Dark field optical microscopy, tapping mode atomic force microscopy, and transmission electron microscopy were used to examine the crystallized film morphologies. At low temperatures, the growth velocity increases with temperature and the morphology consists of a wavy pattern with elongated surface features extending roughly parallel to the crystallization front. TEM observations show this morphology to be a periodic banding of fine and large-grained polycrystalline regions. These structures, coupled with the relatively low average crystallization velocities, suggest a kinetic instability that leads to staggered motion of the crystallization front. At high temperatures, the velocity saturates at a plateau of 14-17 m/s. The morphology consists of columnar-like structures with surface features extending perpendicular to the growth front. Long needle shaped single crystal grains form in this nearly unidirectional pattern. This regime arises from self-selection of a stable, high velocity, growth mode. At intermediate temperatures, explosive crystallization produces a mixed pattern consisting of irregularly arranged patches of surface structures, characteristic of both the low and high temperature regimes. In this transition region, the velocity increases steeply with temperature, and is marked by substantial scatter in average velocities. Average velocities can exceed the ultimate plateau velocity, suggesting the existence of additional unstable, but high velocity, growth modes. Continuum and atomistic modeling of growth in these regimes, to elucidate the underlying physical mechanisms, will also be presented.

P11.13

FABRICATION OF A STRAIN-DISTRIBUTION-CONTROLLED SILICON SURFACE: ANALYSIS OF THE SURFACE BEFORE AND AFTER HOMOEPIITAXY. D.J. Bottomley, H. Omi, and T. Ogino, NTT Basic Research Laboratories, Atsugi, Kanagawa, JAPAN.

Strain distribution control on the Si wafer scale is an important goal because it enables the fabrication and selective positioning of nanostructures. We demonstrate a method for realizing this goal. Oxide inclusions are formed at selected places within the Si bulk by implanting O ions through a SiO₂ pattern. The pattern is removed by HF etching; this is followed by annealing in an Ar atmosphere containing 2% O₂ at 1325°C for 2.5 hours. The volume of the oxide inclusion is approximately double that of its Si content prior to oxygen implantation. The oxide inclusion's stress leads to a strain distribution at the Si surface which can be used for nanostructure fabrication. We have investigated Si(001) and Si(111) wafers implanted with 180 keV O ions. Cross-sectional TEM analysis of the annealed wafers shows faceted oxide inclusions in the bulk, ≈100 nm in diameter, located an average distance of ≈300 nm below the surface. At an implantation density of 2·10¹⁷ cm⁻², the (001) wafer surface is free of defects due to the buried oxide, whereas a few line defects are observed to reach the (111) wafer surface. After the annealing and a HF etch, it was observed in AFM that steps are continuous across the surface, and that the oxide inclusions cause a smooth surface topography ≈10 nm high. The step orientation and spacing change under the influence of the surface strain. For a 2 μm diameter hole array pattern on Si(001), domes ≈10 nm high form above the implantation sites due to elastic deformation of the surface. The surface is also investigated following 100 nm Si homoepitaxial growth, using AFM and micro-Raman spectroscopy. During growth, RHED confirmed film-substrate coherence. AFM demonstrated that the height of the surface topography agreed with that prior to growth, but the step orientation and spacing altered.

P11.14

MOLECULAR DYNAMICS SIMULATIONS OF CRYSTAL GROWTH FROM MELTED Si: GROWTH MECHANISM AND DEFECT FORMATION. T. Motooka and K. Nishihira, Kyushu University, Dept of Materials Science and Engineering, Fukuoka, JAPAN.

Crystal growth processes of Si from the melt have been investigated based on molecular dynamics (MD) simulations using the Tersoff potential. A tetragonal cell with a size of 65.2 Å × 65.2 Å × 43.4 Å composed of 9216 atoms was immersed in a thermal bath with various temperature gradients in the growth direction. After the system reached the stationary state and the solid/liquid interface was obtained, the MD cell was pulled in the [001] and [111] directions with a constant speed for crystal growth. The primary results are as follows: (1) The solid/liquid Si interface was a rough surface composed of {111} facets in the [001] pulling, while it was essentially a flat (111) surface in the [111] pulling; (2) the melt growth in the [001] direction occurred by attaching Si atoms in the melt at the kink sites associated with the {111} facets formed at the solid/liquid Si interface, while in the [111] direction double-layered two-dimensional nucleation was first created and then followed by double-step layer-by-layer growth; and (3) defect formation was initiated by a 5-membered ring composed of a

[110] dimmer bond, like the dimmer on the 2x1 reconstructed Si (001) surface, created at the solid/liquid interface which gave rise to an extended <110> split interstitial. Examples of atomic motions at the solid/liquid interfaces during the melt growth obtained by MD simulations described above will be shown by a movie.

P11.15

Abstract Withdrawn.

P11.16

ORDERING IN AlGaN: THERMODYNAMICAL AND X-RAY ANALYSIS. S. Ruffenach-Clur, O. Briot, M. Moret, R.L. Aulombard, GES, Université Montpellier II, Montpellier, FRANCE.

Up to date, different groups have reported ordering phenomena in nitrides alloys like InGaN or AlGaN. These evidences of ordering during and after growth lead us to study the atomic arrangement of Al and Ga on site III in the AlGaN alloy using a thermodynamical approach. We have defined the enthalpy and the entropy of our system using the Keating model and the cluster variation method limited to the first coordination shell. This study gives us a good way to understand ordering, and moreover to see why at three special compositions (25%, 50% and 75%), the alloy have good chances to present a better crystalline quality than in other cases. In order to verify our hypothesis, we have grown AlGaN samples increasing the Al composition by 10% steps, in the full range of composition from GaN to AlN. All the growth parameters were kept constant except for the alloy composition. X-Ray diffraction measurements performed on these samples indicate that FWHM increases linearly with Al composition, except for three compositions, where according to our thermodynamical study, we observe an improved crystalline quality.

P11.17

MEASUREMENT OF V/III RATIO FOR GaSb/AlSb USING RHEED AND PHOTOEMISSION. J.H.G. Owen, W. Barvosa-Carter and J.J. Zinck, HRL Laboratories LLC, Malibu, CA.

The ratio between the Group V and Group III flux (the V/III ratio) in MBE growth is known to have an impact on the morphological, electrical and optical properties of the grown layers. In the case of arsenide semiconductors, we measure both the Group III and Group V fluxes by using growth oscillations. The response of the RHEED is significantly different in the case of the antimonides compared to the arsenides, necessitating a different approach to the measurement of the V/III ratio. A new method, utilising the sensitivity of the RHEED specular beam intensity to surface reconstruction, is proposed. We see a general correspondence between the RHEED and Photoemission signatures in both cases, so that this method may also be used to measure the average V/III ratio across a large part of a rotating sample.

P11.18

INTERFACIAL ROUGHENING IN GaInP/GaAs HETERO-STRUCTURES. Y.Q. Wang and Z.L. Wang, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA; T. Brown, A. Brown and G. May, Department of Electrical Engineering Georgia Institute of Technology, Atlanta, GA.

Interfacial morphological evolution of solid-source molecular beam epitaxy (MBE) lattice-matched (mismatch strain: 0.093%) GaInP-GaAs heterostructures has been studied by transmission electron microscopy (TEM). Basically, the interfaces exhibit three types of morphologies at micron-scale: planar, irregular roughening and facet roughening. The first several epilayers are found to have planar interfaces, which, however, experience atomic-scale roughening. For the following interfaces, the GaInP-to-GaAs interfaces show irregular roughening on both micron and atomic level. {113} faceted roughening occurs in the GaAs-to-GaInP interfaces, leading to the formation of V-shaped grooves. For GaInP layers exhibiting atomic-scale roughening, a small number of dislocations, mostly 60°-type and in a dipole configuration, are confined in a zone of about 5.0 nm width along the interface, and dislocations are rarely observed deep inside the layers. For GaInP layers with irregular interfacial roughening, in contrast, there is a high density of dislocations in both regions. Based on their distribution and configurations, the dislocations are believed to result from the compositional modulation occurred in the GaInP layers. The interplay of roughening, dislocations and compositional modulation has been discussed in the light of the morphological features.

P11.19

BALLISTIC ELECTRON EMISSION SPECTROSCOPY ON GaAs/AlGaAs SUPERLATTICES. Joonah Yoon, Dept. of Physics, MIT and Gordon McKay Laboratory of Applied Science, Harvard University, Cambridge, MA; Venkatesh Narayanamurti, Gordon McKay Laboratory of Applied Science, Harvard University, Cambridge, MA; Yi-Jen Chiu, Electrical and Computer Engineering

Dept., University of California, Santa Barbara, CA.

BEES (Ballistic Electron Emission Spectroscopy) technique has been employed to study the electron transport through the miniband of GaAs/AlGaAs superlattices at 300 and 4 Kelvin. 10 or 5 period superlattices are grown by MBE below 5.0 or 2.5 nm cap layer of GaAs and thin Au layer was deposited on top of the sample to form a Schottky barrier with GaAs cap layer. BEES data for superlattice structure is compared with those for plain GaAs and GaAs/AlGaAs single barrier structure. This comparison shows that the threshold voltage for miniband of a superlattice lies between the threshold voltage for GaAs Schottky barrier and GaAs/AlGaAs single barrier. In the second derivative of BEES data, the miniband manifests itself as a clear peak. The temperature dependence of the miniband peak location agrees with self-consistent Schrodinger-Poisson calculations of the structure. This work shows that BEES is a good experimental tool to characterize the physics of nanostructures.

P11.20

DYNAMICS OF Ga CLUSTERS ON GaAs(001) SURFACE.

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Dynamics of Ga clusters on a GaAs (001) surface were successfully observed by a scanning tunneling microscopy by a system in which scanning tunneling microscopy (STM) and molecular beam epitaxy (MBE) were equipped with not separated each chambers but one incorporate unit^[1]. With the substrate temperature of 200°C, reflection high-energy diffraction (RHEED) pattern showed a (2x4) As-stabilized surface reconstruction and STM images of steps and a very few islands were clearly observed in constant current mode using sample biases of -3.5V (filled states), tunneling currents of 0.2 nA, and with background pressure of 2x10⁻¹¹ torr. Ga heptamer clusters^[2] moved along the missing dimer row of the (2x4) β 2 surface with keeping its shape and became separated Ga adatoms when it reached B-step edges and moved to the most active sites^[1]. Moreover, with the substrate temperature of 528°C, RHEED pattern showed a (4x6) Ga-stabilized surface reconstruction^[3] and dynamics of steps and islands were clearly observed. The detaching and attaching of small Ga clusters might cause the change of steps and islands. It seems that the small Ga clusters migrated with the diameter of about 0.8 to 1.2 nm and around the steps and islands. These clusters could be observed only when it was detached from or attached to the steps and islands. [1] S. Tsukamoto and N. Koguchi, J. Cryst. Growth 201/202 (1999) 118. [2] S. Tsukamoto and N. Koguchi, J. Cryst. Growth 209 (2000) 258. [3] S. Tsukamoto and N. Koguchi, Jpn. J. Appl. Phys. 33 (1994) L1185; J. Cryst. Growth 150 (1995) 33.

P11.21

INITIAL GROWTH OF EPITAXIAL ZnO ON a-SAPPHIRE.

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High quality, c-oriented ZnO epitaxial films have been grown on the a-surface of sapphire using molecular beam epitaxy. The use of a-oriented sapphire has been shown to eliminate rotational domains and related structural defects present in ZnO grown on c-sapphire which have limited the use of ZnO in electronic applications. In this talk, we present a combination of atomic force microscopy, pole-figure analysis, high-resolution x-ray reciprocal space mapping (HRSM), and EXAFS data to elaborate on the growth mechanisms active during the initial growth process. ZnO films were grown by molecular beam epitaxy onto a-oriented sapphire substrates using a Zn effusion cell and a RF radical cell as sources. After thermal cleaning of the substrate, ZnO layers were grown for 15, 30, 40, 60, and 600 seconds. RHEED observations in-situ indicated the films were epitaxial and c-oriented. Pole figure measurements ex-situ indicated that the ZnO epitaxial layers were uniquely oriented with the ZnO/sapphire orientational relationship [0001] || [1120] and <1120> || [0001] for growth times of 45 s or more, while no in-plane orientation could be seen within experimental error for growth times of 30 s or less. In contrast, HRSM along the surface normal indicated the presence of a narrow mosaic (~ 10 arcseconds) and a ~ 0.3° crystallographic tilt with a distribution of lattice constants from ~ 0.5 nm – 0.54 nm. Short range order changes associated with these surprising large changes in structure are explored with EXAFS measurements using the Zn edge.

P11.22

GROWTH AND CHARACTERIZATION OF CdS/CdTe HETEROJUNCTIONS. Paul Boieriu¹, Robert Sporken^{1,2}, Yan Xin¹,

N.D. Browning¹, S. Sivananthan¹. ¹Microphysics Laboratory, University of Illinois at Chicago, Chicago, Physics Department, IL; ²Facultés Universitaires Notre-Dame de la Paix, Laboratoire

Growth of single crystal wurtzite Cadmium Sulphide on CdTe(111)B substrates has been achieved using molecular beam epitaxy. Cadmium sulfide is a wide band gap semiconductor with $E_g = 2.42$ eV, used mostly as window material for high efficiency solar cells, in tandem with CdTe and CdTe related alloys. Other possible applications include the use of CdS as a window layer for HgCdTe infrared detectors or as an active layer based on the photorefractive effect exhibited in CdS_{1-x}Se_x alloys, suitable for measuring optical frequency differences. Several attempts of growing CdS using molecular beam epitaxy have had their focus on the zinc-blende structure. However, the wurtzite structure is the thermodynamically stable phase. In this work, we have used MBE to grow wurtzite CdS on CdTe(111)B/Si substrates. Cadmium Sulfide can be doped n-type whereas p-type is very difficult due to strong self-compensation. During the growth In has been used as in-situ dopant. Reflection high-energy electron diffraction (RHEED) patterns show a smooth surface morphology for several hundreds of nanometers since the nucleation. X-ray diffraction confirm the crystalline orientation. The epilayers were further characterized by high-resolution TEM, X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES). XPS indicates the existence of a reaction at the interface, the reacted layer being about 10 Å thick. A thin CdTe buffer layer is grown before the growth of CdS. Sulfur incorporation into this CdTe buffer layer has been investigated for various S background pressures. Typically, 5 - 10% S is detected in the CdTe buffer layers. Based on Vegard's law, the shift in the XRD spectra confirms the value of S concentration of these layers. Finally, ohmic and rectifying contacts have been made on these In-doped CdS layers.

P11.23

SUBSTRATE MISORIENTATION AND EXCESS As CONTENT OF LOW TEMPERATURE GROWN GaAs IN RELATION TO STRUCTURAL AND OPTICAL PROPERTIES. Carsten Schuer, Tamas Marek, Michael Becker, Horst P. Strunk, Institute for Microcharacterisation, Friedrich-Alexander-University Erlangen-Nuremberg, GERMANY; Soenke Tautz, Peter Kiesel, Stefan Malzer, Gottfried H. Doehler, Institute for Technical Physics I, Friedrich-Alexander-University Erlangen-Nuremberg, GERMANY; Frank Schroeder, Manfred Niecke, Department of Experimental Physics I, University of Hamburg, GERMANY.

The effect of substrate misorientation on the incorporation of excess As during molecular beam epitaxial (MBE) growth of GaAs at reduced substrate temperature (LT-GaAs) is studied. We examine epitaxial layers grown on GaAs(100) substrates, exactly oriented and tilted up to 10° towards the <111>A resp. <111>B direction. We compare the excess As content, determined by proton induced x-ray emission (PIXE) and secondary ion mass spectroscopy (SIMS), and the structural and optical properties of these layers. The structural properties are examined with transmission electron microscopy (TEM) and high resolution x-ray diffraction (HR-XRD), the optical properties with near band gap absorption measurements. Additionally, we examine the surface morphology with reflection electron microscopy (REM) and atomic force microscopy (AFM). We find a clear influence of substrate misorientation on the excess As content. This result will be discussed in the light of the structural and optical properties.

P11.24

Transferred to P12.3

P11.25

OPTIMIZATION OF LASER ENERGY FLUENCE IN PULSED LASER DEPOSITION OF ZnO ON Al₂O₃(0001). W. Yang¹, R.D.

Vispute, S. Choopun, R.P. Sharma, and T. Venkatesan¹, CSR, Dept of Physics, Univ of Maryland, College Park, MD; ¹also with Electrical and Computer Engineering Dept, Univ of Maryland, College Park, MD.

Pulsed laser deposition (PLD) is a successful technique for congruent transferring composition of bulk oxides into thin films. In this paper, we investigate the influence of laser energy parameter on the growth of ZnO on Al₂O₃(0001). During the PLD process, the laser energy density of a 248nm KrF excimer laser was varied from 1.0 to 2.5 J/cm², while the substrate temperature and oxygen pressure were kept at 750°C and 1x10⁻⁴ Torr, respectively, which were optimized previously [1-2]. The deposited ZnO epilayers have been characterized by various techniques. The scanning electron microscopy (SEM) and atomic force spectroscopy (AFM) morphology pictures show that ZnO films deposited with low laser fluence has hexagonal hillocks well above the surface, while higher laser energy gives flat surface with hexagonal pits. The structural and optical properties, and surface morphology of the films were investigated by x-ray diffraction, Rutherford backscattering spectrometry, photoluminescence (PL) and ultra-violet visible transmission spectroscopy. Electronic properties such as electron concentration and Hall mobility were measured by

the Hall measurements. The results based on different laser energy fluences are compared and correlated with surface morphology, optical, and electronic properties. The issues such as growth mechanisms, defects, surface, and interface of the films will be discussed. [1] Oxygen pressure-tuned epitaxy and optoelectronic properties of laser-deposited ZnO films on sapphire, Choopun S, Vispute RD, Noch W, et al. APPL PHYS LETT 75: (25) 3947-3949 DEC 20 1999. [2] High quality crystalline ZnO buffer layers on sapphire (0001) by pulsed laser deposition for III-V nitrides, R.D. Vispute, V. Talyansky, Z. Trajanovic, S. Choopun, M. Downes, R.P. Sharma, T. Venkatesan, M.C. Wood, R.T. Lareau, K.A. Jones, and A.A. Iliadis., Appl. Phys. Lett. 70, 2735 (1997).

P11.26

DIMER VACANCY LINE DEFECTS ON Si(100) 2x8 SURFACE. Eunja Kim and Changfeng Chen, Dept. of Physics, University of Nevada, Las Vegas, NV.

The dimer vacancy line (DVL) defect on Si(100) surface has been investigated using tight-binding total-energy calculations. To reproduce real scale experimental STM image¹ we use a very large super-cell (32x2), so that the interaction between one DVL and other DVL can be avoided whenever it is necessary. Four DVLs were introduced to study the optimum width of individual DVLs, keeping the defect density at 0.25 ML. There is only attractive interaction between two DVLs while there are both attractive and repulsive interactions for more than three DVLs introduced. The competition between attractive and repulsive interactions plays an important role in determining the optimum width of DVLs. Four DVLs tend to separate into two 2DVL instead of either accumulating at one place forming one 4DVL or four individual single DVLs. This tendency remains even at higher densities of 0.300 ML and 0.375 ML. It implies that introducing more DVLs does not induce larger DVLs with wider widths, but rather narrower distances between DVLs. The experimentally suggested model of dimer line defect, (2 1)DV, is energetically favorable to the 3DVL model.

¹Tsai *et al.*, Phys. Rev. B 56, 7435 (1997).

P11.27

Abstract Withdrawn.

P11.28

THE INFLUENCE OF EMERGENCE POINTS OF DISLOCATIONS ON THE LATERAL MOTION OF GROWTH STEPS ON SOLUTION GROWN GaAs(001) SURFACES. T. Marek, H.P. Strunk, Institute for Microcharacterisation, Friedrich-Alexander-University Erlangen-Nuremberg, GERMANY.

GaAs epitaxial layers are grown from Ga-solution onto spherically shaped GaAs(001) substrates (liquid phase epitaxy, LPE). The spherical shape ensures vicinal surfaces with deviations of up to 2 degree off [001].

After growth, the surfaces are investigated by optical microscopy (Nomarski differential interference contrast, NDIC). Selected areas are investigated by reflection electron microscopy (REM). In the region around the exact 001 orientation ($\pm 0,1$ degree) a very smooth facet develops containing monosteps only. This topology indicates growth of the layer by layer growth. This facet region is surrounded by a terraced area. In this terrace region growth occurs by the motion of steps up to 10 to 15 elementary step in height. We find in both, facet and terrace region that the emergence points of dislocations block the lateral motion of the growth steps. This lead in the terrace region to formation of pronounced depressions elongated in the lateral growth direction, that are reminiscent of tailbacks. Details of these structures and their dependencies on the growth conditions will be discussed in terms of a microscopic model.

P11.29

PATTERN EVOLUTION OF NiSi₂ ON A Si SURFACE UPON HIGH CURRENT PULSED Ni ION IMPLANTATION. H.N. Zhu and B.X. Liu, Tsinghua Univ, Dept of Materials Science and Engineering, Beijing, CHINA.

Fractal pattern evolution of NiSi₂ grains on a Si surface was induced by high current pulsed Ni ion implantation into Si using metal vapor vacuum arc ion source [1,2]. The fractal dimension of the patterns was found to correlate with the temperature rise of the Si substrate, which was self-heated by the implanting Ni ion beam. With increasing of the substrate temperature, the fractal dimensions were determined to increase from less than 1.64 being approximately the value of cluster-diffusion-limited-aggregation (CDLA), to beyond the percolation threshold of 1.88, and eventually up to a value of 2.0, which corresponded to a uniform NiSi₂ layer with fine grains applicable in the electronic devices. Meanwhile, a pre-deposited Ni-overlayer on the Si surface was found to have some influence on the growth of the fractal patterns. With increasing the thickness of the Ni overlayer, the fractal dimension increased a little, yet the

characteristics of the corresponding patterns did not change. In addition, the measured sheet resistance of the Si surface varied in a well compatible way in accordance with the variation of the fractal dimensions. The growth kinetics of the observed surface fractals was also discussed in terms of the special launching mechanism of the Ni ions into the Si wafers as well as the interactions among the Ni and Si atoms at elevated temperature upon pulsed Ni ion implantation. Consequently, the growth of the fractal pattern on a Si surface was attributed to a process named as intermittent CDLA.

References:

1. K.Y. Gao and B.X. Liu, J. Phys. Condensed Matter 11, 39 (1999).
2. H.N. Zhu, K.Y. Gao and B.X. Liu, Phys. Rev. B (July 15 issue, 2000).

P11.30

DIFFUSION AND REACTION KINETICS OF NIOBIUM/GOLD THIN FILMS FOR FIRST LEVEL DEVICE INTERCONNECTS.

Robert Esser, Aris Christou, Dept. of Materials Science and Engineering, University of Maryland-College Park, College Park, MD.

Auger electron spectrometry depth profiles, sheet resistance measurements, and x-ray diffraction have been used to investigate the diffusion kinetics of electron beam evaporated Nb/Au thin films. Niobium/gold thin films were deposited on thermally oxidized silicon substrates and annealed isochronally at temperatures ranging from 200 to 500 degrees Celsius and for 8 to 672 hours isothermally. A model to simulate and understand the intermetallic growth at the interface of the films has been applied. Diffusion coefficients and activation energies have been measured. Transmission Electron microscopy shows that significant resistivity changes do not occur until all of the niobium has been reacted with gold to form Au₂Nb intermetallic compound. Sheet resistance increases were directly attributed to the formation of the Au₂Nb phase. Temperature processing parameters and possible temperature profiles for device applications have been determined.

P11.31

TiNi/GaAs THIN FILM STRUCTURES FOR GATE METALLIZATIONS. Chichang Zhang, Aris Christou, Dept. Materials Science and Engineering, Univ. of Maryland, College Park, MD.

The shape memory alloy TiNi thin films on GaAs have been investigated for high frequency applications in order to take advantage of the piezoelectric phenomena in GaAs. A series of TiNi compositions were electron beam deposited on GaAs initially as thin multilayers of Ti and Ni. The intermetallic phase of TiNi was formed by annealing and completely intermixing the multilayers at 370°C. The intermetallic phases were investigated with x-ray diffraction techniques. The annealing kinetics and resistivity investigations were carried out in order to minimize the sheet resistance of the intermetallic phase. GaAs MESFETs with TiNi Schottky barriers have been fabricated and performance will be reported. Additional investigations on surface morphology using the scanning electron microscope as well as TEM investigations show the correlation between microstructure, intermetallic phase formation and sheet resistance.

P11.32

IMPROVEMENT OF THIN PALLADIUM SILICIDE FILMS ON (100) SILICON SUBSTRATES BY INCORPORATING PHOSPHORUS DOPANT. Miin-Horng Juang, Chan-I Ouyang, National Taiwan University of Science and Technology, Dept of Electronic Engineering, Taipei, TAIWAN; Huang-Chung Cheng, Cheng-Tung Lin, National Chaio-Tung University, Dept of Electronic Engineering, Hsin-Chu, TAIWAN.

The self-aligned silicide technology has become an essential part of the fabrication process for ultra-high-speed CMOS logic LSI circuits. Previously, several schemes have been used to form silicided shallow junction. However, the incorporation of dopant into the silicide layer may influence the thermal stability and the crystallinity of the resultant thin silicide films on Si substrates. Effects of phosphorus dopant on the thermal stability of thin Pd and Pt silicide films on (100) Si substrates have been studied. As for the samples formed by implanting BF₂ dopant into thin Pd films deposited on Si substrates and then annealing, the thermal stability of thin Pd₂Si films can be improved relative to the control samples without dopant incorporation. The degree of improvement is affected by the fluorine concentration around the silicide/Si interface and thus the BF₂ implantation energy. On the other hand, as for the samples formed by implanting phosphorus dopant into thin Pd films and then annealing, both the thermal stability and the silicide conductivity of thin Pd₂Si films can be significantly enhanced. The control samples show a large increase of sheet resistance from about 10 Ω/sq. to about 250 Ω/sq. as the annealing temperature is raised from 600 to 700°C, correspondingly. However, for the phosphorus-implanted Pd samples, the sheet resistance of thin silicide films is maintained to be only

about 6 Ω/sq. even if the annealing temperature is raised to 700°C. The large improvements in the thermal stability and the silicide conductivity are nearly independent of the phosphorus implant energy, and thus the previously proposed mechanism to explain the fluorine effect can not account for the influence of phosphorus dopant. Accordingly, it is found that these results are primarily due to the formation of textured Pd₂Si structure. In addition, the Pt silicides formed by implanting phosphorus dopant into thin Pt films and then annealing also similarly show considerably improved thermal stability.

P11.33

EFFECTS OF SILICON SURFACE HYDROGENATION ON INITIAL REACTION PROCESSES OF TRANSITION-METAL ADATOMS. Shin'ichi Higai, Takahisa Ohno, Natl Res Inst for Metals, Tsukuba, JAPAN.

We studied the effects of the surface hydrogenation on the adsorption, surface diffusion, penetration, and silicidation, i.e., the initial reaction processes of the 3d transition-metal Ti and Ni adatoms on the Si(001) surface, based on the first-principles theoretical calculations. It was found that the effects for Ti and Ni are qualitatively identical. First, for the adsorption, the surface hydrogenation changes their most stable surface site from the site on the Si dimer row to that between the dimer rows, and moreover, reduces the adsorption energy. Next, for the surface diffusion, the surface hydrogens suppress it. Third, for the penetration, both Ti and Ni are stabilized by penetrating into the bare Si subsurface, while they do not penetrate into the H-terminated Si subsurface. Their stability in the bare Si subsurface is due to the existence of the dangling-bond charge of the surface Si atoms. We concluded that the surface hydrogenation blocks their penetration, and thus prevents the silicidation. Furthermore, an interesting effect was predicted from our results, that is, Ti and Ni pre-penetrated in the bare Si subsurface are extracted onto the surface by the surface hydrogenation. The dimer vacancy defects seen on the bare Si(001) surface are mainly caused by the contamination by the metallic impurities, especially Ni. Therefore, it is expected that the application of this effect makes it possible to obtain the highly pure and atomically flat Si surfaces.

P11.34

SURFACTANT MEDIATED GROWTH OF MnSi_{1.7} ON Si(001). S. Teichert, H. Hortenbach, A. Mogilatenko, M. Falke, G. Beddies, H.-J. Hinneberg, University of Technology, Chemnitz, GERMANY.

Surfactant mediated film growth has drawn extensive attention since the pioneering works in the system Si/Ge. Much less attention has been paid to the surfactant mediated growth of silicide on Si although there are interesting fields of application using surfactants for the growth of epitaxial layers or silicide silicon multilayers. Among the semiconducting silicides there are the manganese silicides with a composition close to MnSi_{1.7} which are called higher manganese silicides (HMS). The HMS differ slightly in the lattice positions of the Si atoms resulting in a small variation of the Si content, but all reported HMS have a similar tetragonal crystal structure. In this paper we report on the growth of HMS by reactive deposition of Mn on Si(001) using Sb as a surfactant. Under UHV conditions growth was performed by simultaneous or consecutive exposure of the Si substrates, held at high temperatures (550°C, 600°C), to Sb and Mn atoms. It is found that the presence of Sb during the growth strongly increases the island density and changes the crystalline orientation of the HMS. The morphology and structure of the resulting silicide are the same both for the deposition of Mn only on a Sb-terminated Si(001)-surface and for the codeposition of Mn and Sb on Si(001). A residual Sb coverage close to one monolayer at the sample surface has been determined for both of the preparation conditions. The variation of Sb coverage from 0 to about 1 ML (1 ML = 6.78x10¹⁴ atoms cm⁻²) of the Si(001) substrate before deposition of Mn allows a scaling of the silicide island density over two orders of magnitudes.

P11.35

EPITAXIAL IRIIDIUM FILM GROWTH ON STRONTIUM TITANATE. Z. Dai, A.P. Li, C. Bednarski, and B. Golding, Center for Sensor Materials and Department of Physics & Astronomy, Michigan State University.

Epitaxial (100) iridium films have been successfully grown on (100) SrTiO₃ (STO) substrates via UHV electron beam evaporation. The epitaxial relationship between iridium films and STO substrates, as determined by RBS (Rutherford Backscattering Spectrometry)/Channeling, is Ir(100)//STO(100), Ir(110)//STO(110), and Ir(111)//STO(111). Our best epitaxial iridium films are characterized by small Ir(200) rocking curve FWHM (full width at half maximum) < 0.3°, smooth surfaces with mean surface roughness 2Å, and low ion channeling yields, 3%. The dependence of crystalline quality and surface morphology on film thickness, substrate surface condition, and substrate deposition temperature have been studied by X-ray diffraction, RBS/channeling, SEM, electron backscattering, and AFM.

Crystalline quality and surface smoothness depend on film thickness, with improvement as the film thickness increases up to 500 nm. We have found that epitaxial iridium films can only be obtained on substrates with in-situ heating treatments before deposition, and films grown on terraced substrates show narrower rocking curves.

P11.36

SMOOTHENING OF (001) AND (111) Cu FILMS EPITAXIALLY GROWN ON Si SUBSTRATES. R.A. Lukaszew, C. Uher, R. Clarke, Physics Department, University of Michigan.

We have shown recently that it is possible to achieve dramatic smoothening of epitaxial Cu (001) oriented films grown on hydrogen terminated Silicon substrates, through mild annealing steps in at temperatures range below significant silicide formation at the surface ($395\text{K} < T < 445\text{K}$). [1] We found in this temperature interval a lower activation energy ($0.4 \pm 0.03\text{ eV}$) than the reported value of 1.1 eV for (001) Copper in the temperature range $333\text{K} < T < 368\text{K}$. [2] In order to clarify the origin of this significant smoothening, we have studied the MBE (molecular beam epitaxy) growth and annealing of Cu (111) films grown on 7×7 reconstructed Si (111) substrates (hydrogen-free interface). We have observed the evolution of the surface using correlated in-situ RHEED (reflection high-energy-electron diffraction) and STM (scanning tunneling microscopy) measurements. We have found that annealing the films in a temperature interval below silicide formation on the surface, leads to improvement of the film roughness despite the somewhat high activation energy (1.1 eV) measured for mass transport. Our findings also indicate that the absence of a dramatic smoothening when annealing the (111) Cu films, as compared with our earlier reported behavior for (001) Cu films grown on H-terminated (001) Silicon is related to lack of H-termination at the Cu-Si interface. [1]. R.A. Lukaszew, Y. Sheng, C. Uher and R. Clarke, Appl. Phys. Lett. 76, 724 (2000). [2]. J.-K. Zuo and J.A.F. Wendelken, Phys. Rev. Lett. 70, 1662 (1993).

P11.37

ELECTROMIGRATION IN EPITAXIAL Cu LINES. Harmeet S. Goindi, M.J. Frederick, and G. Ramanath, Materials Sci. & Eng. Dept., Y. Shusterman, Physics Dept., Rensselaer Polytechnic Institute, Troy, NY; C.-S. Shin and I. Petrov, Materials Research Laboratory, University of Illinois, Urbana, IL.

Copper has replaced aluminum as the interconnect metal in integrated circuits due to its higher electromigration resistance and lower electrical resistivity. While it is generally accepted that large-grains and (111) texture inhibits electromigration in Al lines, there is no consensus on the effects of grain size and distribution, and preferred orientation on electromigration in Cu. In this paper, we investigate epitaxial Cu structures in order to delineate the effects of grain orientation, size, and morphology on the electromigration mechanism. Epitaxial Cu layers with (111) and (001) orientations were deposited by molecular beam epitaxy (MBE) on Si(111) wafers, and by DC magnetron sputtering on MgO(001) wafers, respectively. $1\text{-}\mu\text{m}$ -wide Cu lines, created from the blanket films by standard lithography techniques, are subject to electromigration tests at constant current densities of $1\text{-}15\text{ MA/cm}^2$ in an Ar ambient at temperatures between 150 and 350°C . The mean time to failure and electromigration activation energy of epitaxial copper lines are compared with that of polycrystalline Cu, and the differences are explained in terms of the grain size and orientation. We will also describe the influence of Ta, TaN and TiN underlayers on electromigration.

P11.38

EPITAXIAL Al AND Cu FILMS GROWN ON $\text{CaF}_2/\text{Si}(111)$. Y.V. Shusterman, N.L. Yakovlev, L.J. Schowalter, Rensselaer Polytechnic Institute, Department of Physics, Troy NY; K. Dovidenko, SUNY-Albany, Center for Advanced Thin Film Technology, Albany NY.

Having an epitaxial metal is beneficial for investigations of electron scattering at metal boundaries and for electromigration failure analysis of VLSI interconnects. Here, we study the epitaxial growth of Al and Cu on $\text{CaF}_2/\text{Si}(111)$. The CaF_2 allows to insulate the metal from the silicon for electrical characterization. Reflection high energy diffraction (RHEED) indicated that the Al films grew epitaxially in 111 orientation despite the large (about 25%) lattice mismatch. Most of the Al appeared to be growing either in the same azimuthal orientation as CaF_2 or twinned around the surface normal. About one fifth of Al also formed domains rotated 30° with respect to the main part of the film. The growth proceeded through formation of 3-dimensional islands that then coalesced as the thickness increased. Using an Al deposition rate above 1 nm/s at room temperature, we were able to obtain continuous films as thin as 10nm with roughness less than 2nm , as measured by atomic force microscopy. Scanning tunneling microscopy showed atomic steps, some of them originating at screw dislocations. The density of these dislocations was around $10^{11}/\text{cm}^2$. Measurements of the Al resistivity as a function of film

thickness showed a clear size effect below about 30nm . The Cu was polycrystalline when deposited directly on CaF_2 , but grew epitaxially when an Al seed layer thicker than 3nm was used. From transmission electron microscopy measurements, we confirmed the epitaxial nature of the films. In case of room temperature growth, RHEED showed that the domain structure of Cu was similar to that of Al. The growth was 3-dimensional, and some polycrystalline Cu formed after deposition of approximately 100nm thick layer. For Cu growth at temperatures above 100°C , the 30° -domains disappeared, the surface became considerably smoother, and no polycrystalline material formed even beyond 200nm thickness.

P11.39

PLASTIC DEFORMATION IN COPPER THIN FILMS STUDIED BY BULGE TESTING. S. Ziegler^{1*}, R. Spolenak¹, W.L. Brown¹, C.A. Volkert², M.L. Peabody¹, R.A. Boie¹, ¹Bell Labs/Lucent Technologies, Murray Hill, NJ; ²I.Physikal.Inst.A, Lehrstuhl für Physik Neuer Materialien, Aachen; ²Max-Planck-Institute fuer Metallforschung, Stuttgart.

In order to systematically study mechanisms of plastic deformation in copper films we have developed a new bulge tester apparatus capable of running at temperatures up to 300°C . Unlike wafer curvature measurements, this apparatus allows the independent application of temperature and stress to the sample. Sputtered and electroplated Cu films were deposited on SiN_x coated silicon substrates with and without Ta or TaN barrier layers. The films were made into membranes by selective crystallographic etching of the silicon with hot KOH to form rectangular $2\text{mm} \times 12\text{mm}$ membranes. The mechanical properties of the composite membranes were investigated using two techniques: 1) resonant frequency measurements under vacuum were used to determine the initial tensile stress, and 2) capacitive measurements of bulge height vs argon gas pressure were used to determine the stress-strain behavior. For example, in $1\text{ }\mu\text{m}$ thick Cu sputtered films the frequency of the lowest resonance mode gave a tensile stress of approximately 200 MPa . Evidence for plastic deformation of the Cu films was observed by both techniques at strains as low as 0.02% . During straining to approximately 0.2% work hardening leading to a yield stress increase of about 100 MPa was observed. Creep has been measured with high instrumental stability at applied stresses between 200 and 400 MPa over many hours with a strain rate sensitivity $< 3 \times 10^{-9}$. Results and interpretation will be presented for the different types of Cu films, annealed and as-deposited and as a function of temperature.

P11.40

ANOMALOUS RHEED OSCILLATIONS DURING INITIAL EPITAXIAL GROWTH OF REFRACTORY TRANSITION METALS ON OXIDE SUBSTRATES. Paul Ryan and Frank Tsui, University of North Carolina, Dept of Physics and Astronomy, Chapel Hill, NC.

Molecular beam epitaxial (MBE) growth of refractory transition metal overlayers on oxide substrates has been studied using real-time reflection high energy electron diffraction (RHEED) and in-situ scanning probe microscopy (SPM). Aperiodic RHEED specular intensity oscillations have been observed. For example, the RHEED specular reflectivity during Nb (111) growth on sapphire (0001) undergoes maxima at 1 and 3 ML, indicating preferential smoothening at these thicknesses; growth of Nb (110) on sapphire, on the other hand, exhibits only one such peak at 1 ML. Growth of Mo (111) on sapphire exhibits a peak at 5 ML instead. While the coverages at which the RHEED specular peaks occur depend sensitively on overlayer/substrate materials and orientations, the peak intensities are influenced strongly by the growth conditions. These features indicate the complex nature of MBE growth of metal overlayers on insulating substrates, and the importance of interplay between energetics and kinetics, particularly the effects of electronic structures of the materials involved.

P11.41

KINETICS OF GRAIN COARSENING IN GOLD THIN FILMS WITH THE MAZED BICRYSTAL STRUCTURE. Tamara Radetic, Ulrich Dahmen, NCEM, Lawrence Berkeley National Lab, Berkeley, CA.

Thin films of Au have been grown by physical vapor deposition on single Ge and Si substrates. The resulting microstructure is that of a mazed bicrystal in which two equivalent grain orientations are related to each other by a 90° rotation. The morphology of the films is characterized by its irregularly shaped, convoluted structure. Quantitative morphological analysis shows a strong dependence of grain shape on size, with larger grains being more convoluted and smaller grains more compact. Due to capillarity forces acting on the curved interfaces there is a tendency of grain boundaries to straighten themselves in order to minimize curvature and decrease the area of the interface. The kinetics of grain growth has been studied by in-situ experiments and the influence of surface grooves on mobility of grain

boundaries has been examined. The effect of annealing on the structure and morphology of the grain boundaries has been characterized by conventional and high resolution electron microscopy. Abnormal grain growth, observed at the specific locations in the film, is discussed in terms of diffusion induced grain boundary migration. This work is supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-ACO3-76SF00098.

P11.42

CONTROL OF GRAIN BOUNDARY LOCATION IN A CRYSTALLIZED Si FILM ON A GLASS SUBSTRATE BY PULSE LASER BEAM WITH LINEAR POLARIZATION. Yasunori Nakata and Susumu Horita, JAIST (Japan Advanced Institute of Science and Technology, Hokuriku).

The pulse laser annealing (PLA) method is effective to produce the polycrystalline silicon (poly-Si) films with the high carrier mobility on a glass substrate. In order to reduce the grain boundary and control its location, it is necessary to control the temperature distribution in the melted Si film. So, we attempted the PLA crystallization with a linearly polarized laser beam, for the first time, which induces the periodic temperature distribution on the surface precisely. A 45- to 110-nm-thick a-Si film deposited on a Pyrex glass substrate at 350°C was irradiated by a Nd:YAG pulse laser beam at the same temperature in the ultra high vacuum chamber. The wavelength, total power and pulse number of the laser beam were 532 nm, 750-1000 mW and 2-5, respectively. In a Secco etched crystallized Si film, it was observed by SEM that the grain boundaries were aligned with the period of about 550 nm or the wavelength of the laser. This means that the grain boundary location is controlled by the periodic temperature distribution without additional process and optical components. The periodic grain boundary direction was perpendicular to the electric field. Also, when the irradiation beam passed through the half-wave plate, the boundary direction was rotated by 90° because the beam polarization was rotated. Further, we observed by XRD measurement that under the constant beam power of 750 mW the crystallized Si film becomes more (111)-oriented with increasing the film thickness from 60 nm whose film was almost randomly oriented. We found a good negative-correlation between the XRD peak intensity of the Si(111) and the calculated absorptivity per unit thickness of the a-Si film. Therefore, it can be inferred that the orientation of the Si film crystallized on the Pyrex glass by PLA depends on the heat source density in the film and that less heating induces (111)-orientation.

SESSION P12: SEMICONDUCTOR EPITAXY

Chair: Karsten Horn

Friday Morning, December 1, 2000

Room 302 (Hynes)

8:30 AM P12.1

ATOMIC STRUCTURE OF GaAs(2511) - A NEW STABLE SURFACE. Lutz Geelhaar, Juan Márquez, Peter Kratzer, Karl Jacobi, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, GERMANY.

A new stable GaAs surface has been discovered whose orientation is (2511). Samples were prepared by molecular beam epitaxy (MBE), and the atomic structure of this new surface has been determined on the basis of *in situ* scanning tunneling microscopy (STM) measurements and first-principles electronic structure calculations. This is the first demonstration that a stable surface of a III-V-semiconductor exists inside the stereographic triangle, i. e. far away from the low-index surfaces (100), (110) and (111). A (1×1) reconstruction containing arsenic dimers forms on the surface. Terraces extend over more than 1000 Å. The surface structure is perturbed by regular stripes that are several 100 Å long but only 13 Å wide. This long-range, ordered violation of the periodicity is due to the semi-stability of GaAs(3715), a nearby surface. The analysis of this phenomenon yields an increased understanding of the general principles for the surface structure of compound semiconductors. Because of the different electronic structures of these two surfaces it is speculated that the stripes constitute one-dimensional systems. The relevance of the new stable surface is shown by further STM experiments on InAs/GaAs(001) quantum dots. The shape of these three-dimensional islands comprises facets whose structure is closely related to that of GaAs(2511).

8:45 AM P12.2

OBSERVATION OF SPONTANEOUS VERTICAL COMPOSITION MODULATION IN EPITAXIAL GaInAsSb. C.A. Wang, C.J. Vineis, D.R. Calawa, P.M. Nitishin, Lincoln Laboratory, Massachusetts Institute of Technology, Lexington, MA.

Spatial variations in the alloy composition of ternary and quaternary III-V semiconductor alloys can result from phase separation or strain. Both lateral and vertical composition modulation have been observed in several materials systems, although lateral modulation is far more commonly reported. In this work, observations of spontaneous vertical composition modulation in epitaxial $\text{Ga}_{1-x}\text{In}_x\text{As}_y\text{Sb}_{1-y}$ ($0 < x < 0.2$, $0 < y < 0.2$) is reported. These alloys have a large miscibility gap, but still can exhibit excellent materials properties, and high-performance thermophotovoltaic devices have been reported. Nominally lattice matched layers are grown by organometallic vapor phase epitaxy on (001) GaSb substrates miscut 2 or 6° toward (-1-11)A, (1-11)B, or (101). Field emission scanning electron microscopy and transmission electron microscopy (TEM) of layer cross-sections reveal a layered structure with a high degree of regularity in the growth direction. The layers are continuous and straight over several microns of lateral distance, and spontaneously form a highly regular superlattice. It is reproducible and is observed for a wide range of substrate miscuts, alloy compositions, and deposition temperatures (525 to 575°C). The periodicity of the modulation is dependent on deposition temperature and alloy composition, and is typically between 15 to 20 nm. Cross-section TEM suggests that GaInAsSb self-organizes at the onset of growth and maintains a consistent periodicity throughout several microns of deposition. Triple-axis x-ray diffraction is used to map the reciprocal space structure and provides a quantitative measure of the magnitude and direction of lattice tilt. A particularly remarkable feature of the vertical modulation is the ordering of atoms to produce a layered structure that is tilted 4° in addition to the miscut angle of the (001) substrate surface plane. Atomic force microscopy of the surface step structure shows that it is vicinal or step-bunched, depending on the growth temperature. Possible mechanisms for the formation of these structures are discussed.

9:00 AM P12.3

SURFACE ROUGHENING AND INTERFACIAL BOND FORMATION DURING ARSENIDE AND ANTIMONIDE HETEROEPITAXY. Brett Z. Noshov, Allan S. Bracker, Brian R. Bennett, Ming-Jey Yang, Benjamin V. Shanabrook, and Lloyd J. Whitman, Naval Research Laboratory, Washington, DC.

The 6.1 Å family of compound semiconductors, InAs, GaSb, and AlSb, provides the basis for a wide variety of novel device heterostructures. In order to optimize and reproducibly fabricate high-quality devices, it is critical to understand, characterize, and ultimately control the complex interplay between kinetics and thermodynamics that occurs during epitaxial growth and interface formation. We have combined scanning tunneling microscopy (both plan-view and cross-sectional) with reflection high-energy electron diffraction (RHEED) to study the evolving surface morphology and the associated interfacial structure in 6.1 Å heterostructures grown by molecular beam epitaxy (MBE). Interfacial disorder is created when islands are kinetically trapped during growth and/or when components segregate or exchange across the interface. We will show how abrupt changes in surface reconstruction during growth may cause spontaneous island formation. Because several different III-Sb reconstructions exist within the range of typical device growth conditions, this roughening can occur even during homoepitaxy, affecting the island size distributions and shifting the phase of the RHEED oscillations during subsequent growth. We will also report on our ongoing studies of roughness associated with interfacial bond formation for both InSb-like and (Ga,Al)As-like bonds, and discuss how exchange reactions depend on growth temperature and group V species (e.g. As₂ vs. As₄). Supported by DARPA and ONR.

9:15 AM P12.4

IN SITU OBSERVATION OF FACETING OF VICINAL GaAs(001) INDUCED BY SILICON. S. Brennan, SSRL/SLAC, Stanford, CA; G.B. Stephenson, Argonne National Laboratory, Argonne, IL; P.H. Fuoss, AT&T Laboratories, Florham Park, NJ; D.W. Kisker, Cielo Communications, Inc, Broomfield, CO; C. Lavoie, IBM Research, Yorktown Heights, NY; K.L. Evans-Lutterodt, Lucent Technologies, Murray Hill, NJ.

We present *in situ* x-ray diffraction studies of the changes in the morphology of 0.5°-miscut vicinal GaAs(001) surfaces during and after undoped and silicon-doped growth using organo-metallic vapor-phase epitaxy (OMVPE). Undoped growth results in ordered monolayer steps. However, growth in the presence of silicon destabilizes this surface morphology and triggers faceting. These facets continue to enlarge even after the growth has stopped and results in large regions of singular GaAs(001) surface separated by regions of step bunches. Both doped growth and undoped growth following silicon dosing results in the development of facets, but dosing the surface with silicon without growth does not result in faceting. Growth of undoped GaAs on faceted surfaces recovers the initial state of ordered monolayer steps.

9:30 AM P12.5

DEFORMATION BEHAVIOR OF THIN BUFFER LAYERS IN STRAINED-LAYER SEMICONDUCTOR HETEROEPITAXIAL GROWTH. Dimitrios Maroudas, Luis A. Zepeda-Ruiz, Rodney I. Pelzel, and W. Henry Weinberg, Dept. of Chemical Engineering, Univ. of California, Santa Barbara, CA.

In strained-layer heteroepitaxial growth, the biaxial strain induced in the epitaxial film due to its lattice mismatch with the substrate is a major factor in determining the film's structural quality and electronic properties. Processing strategies for elastic accommodation of the strain in the film by a finite-thickness substrate are particularly promising for stress control and property optimization in semiconductor heterostructures. In this presentation, we examine both theoretically and experimentally the deformation behavior of coherently strained semiconductor heteroepitaxial systems consisting of thin buffer layers and layer-by-layer grown epitaxial films. A systematic, quantitative analysis is presented of the mechanical behavior of coherently strained InAs/GaAs heteroepitaxial systems. Our analysis combines a hierarchical theoretical approach with experimental measurements. Continuum linear elasticity theory is linked with atomic-scale simulations of structural relaxation for detailed theoretical studies of deformation in systems consisting of InAs thin films on thin GaAs(111)A substrates that are mechanically unconstrained at their bases. Molecular beam epitaxy is used to grow very thin InAs films on both thick and thin GaAs buffer layers on epi-ready GaAs(111)A substrates. The deformation state of these samples is characterized by X-ray diffraction (XRD). The interplanar distances of thin GaAs buffer layers along the [220] and [111] crystallographic directions obtained from the corresponding XRD spectra indicate clearly that thin buffer layers deform parallel to the InAs/GaAs(111)A interfacial plane, thus aiding in the accommodation of the strain induced by lattice mismatch. The experimental measurements are in excellent agreement with the calculated lattice interplanar distances and the corresponding strain fields in the thin mechanically unconstrained substrates considered in the theoretical analysis. Therefore, this study contributes direct evidence supporting that thin buffer layers in layer-by-layer semiconductor heteroepitaxy exhibit mechanical behavior similar to that of thin compliant substrates.

9:45 AM P12.6

THE NATURE OF ISLANDING IN THE InGaAs/GaAs EPITAXIAL SYSTEM. Thomas Walther, Institut für Anorganische Chemie, Universität Bonn, Bonn, GERMANY; Antony G. Cullis, David J. Norris, Mark Hopkinson, Dept. Electronic and Electrical Engineering, University of Sheffield, Sheffield, UNITED KINGDOM.

There is great interest in the phenomenon of islanding in a range of semiconductor systems, in part due to the fundamental importance of the Stranski-Krastanow transition but also strongly driven by potential device applications of (self-organised) quantum dot arrays. However, the mechanisms underlying the island formation transition are still to a significant degree unclear and require a better understanding to be obtained. In the present work, we address these issues and focus on the epitaxial InGaAs/GaAs system, with layer deposition by molecular beam epitaxy. The structure of such layers during early stages of growth is examined using transmission electron microscopy and detailed, nano-scale compositional measurements are made by state-of-the-art electron energy-loss imaging. Indium gradients in the islanded layers are measured and the driving force for the islanding transition itself is considered.

10:30 AM P12.7

MECHANISM OF INTERFACIAL COARSENING IN MOLECULAR BEAM EPITAXY GROWTH ON (001) CRYSTALLINE SURFACES. Leonardo Golubovic, Department of Physics, West Virginia University, and Dorel Moldovan, Materials Science Division, Argonne National Laboratory.

We theoretically address epitaxial growth on crystalline surfaces with square symmetry, in the regime when pyramids are formed across the growing interface due to Schwoebel-Ehrlich-Hudda step-edge barriers. We develop a kinetic scaling theory that analytically explains numerous experiments and simulations suggesting that pyramid size grows, via coarsening, as a fourth root of the deposition time. Pyramid dynamics is elucidated in terms of pyramid edges that form growing self-organized square lattice across the growing interface. The edge lattice of pyramids is disordered by topological defects that are characterized here as dislocations. We show that pyramid coarsening is mediated by climb-motion of the dislocations of the edge lattice. By taking into account this motion as well as the processes of dislocation annihilations, we can analytically explain the experimentally observed power law growth of pyramids on (001) crystalline surfaces, as well as a multi-scaling growth seen in simulations.

10:45 AM P12.8

DISLOCATION PATTERNING IN PbTe HETEROEPITAXY ON PbSe (100) SUBSTRATES. Karin Wiesauer and Gunther Springholz, Johannes Kepler Universitaet, Linz, AUSTRIA.

Molecular beam epitaxy of PbTe on 5.2% lattice-mismatched PbSe (100) substrates is studied using scanning tunneling microscopy. It is found that at a critical layer thickness of 0.8 monolayers, pure edge type misfit dislocations are formed at the layer/substrate interface. In the STM images these misfit dislocations appear as dark lines (local surface depressions) that run over the epitaxial surface along the four-fold $\langle 011 \rangle$ directions. From atomically resolved lattice images, the dislocation Burgers vector is found to be $1/2 \langle 001 \rangle$ parallel to the interface. This unusual misfit dislocation configuration is explained by the fact that the easy dislocation glide planes in the lead salt compounds are either perpendicular or parallel to the (100) interface. As a consequence, misfit dislocations cannot be formed by glide but only by climb processes. From a detailed STM investigation of the very early relaxation stages, we find that all misfit dislocations are all injected from monolayer step edges on the surface, which greatly reduces the nucleation barrier of dislocation half loops. As the PbTe layer thickness increases, the misfit dislocation density drastically increases and a nearly perfect quadratic grid of misfit dislocations with an average spacing of around 100 Å is formed, indicating that at 10 monolayers layer thickness more than 90% of the misfit strain is relaxed by dislocations. In addition, the course of strain relaxation is found to be in well agreement with the Frank-van-der-Merwe model. This surprising result is explained by the reduction of the dislocation nucleation barrier by the edge injection mechanism. The remarkable uniformity of the dislocation array is evidenced by the appearance of satellite peaks in the FFT power spectra of the STM images due to the dislocation superstructure. From a statistical analysis we find a variation of the lateral dislocation spacing of only $\pm 10\%$, which is better than the typical size uniformity of self-assembled quantum dots. Thus, these structures could serve as templates for the deposition of self-organized ordered nanostructures.

11:00 AM P12.9

KINETIC PROCESSES DURING GALLIUM NITRIDE NUCLEATION BY ION- AND PLASMA-ASSISTED MOLECULAR BEAM EPITAXY. R.L. Headrick, O. Malis, J.D. Brock, Cornell University, Ithaca, NY.

The nucleation of GaN on (0001) sapphire has been studied by real-time x-ray scattering techniques at the Cornell High Energy Synchrotron Source (CHESS). We have found that the nucleation of the first monolayer of GaN is dramatically enhanced by a nitrogen plasma beam. This effect was originally thought to be due to the enhanced reactivity of nitrogen atoms, ions, or excited species. However, we have recently discovered that a very similar effect is obtained by growth from thermal ammonia when an external beam of low-energy (< 30 eV) Ar ions are directed at the substrate. Control experiments indicate that the effect is due to Ar interactions with the growth surface and critical nuclei during the very early stages of nucleation. We are developing a model for this process based on the effect of ions breaking apart 2D islands. Related experiments show that only a single monolayer "buffer layer" is needed for the growth of high-quality thin films. Subsequent x-ray standing wave measurements on these films to determine the polarity show that the films are nitrogen face GaN.

11:15 AM P12.10

BALLISTIC ELECTRON EMISSION MICROSCOPY ON A SINGLE MONOLAYER Pb/Si(111). I. Altfeder, P. Evans, V. Narayanamurti, J. Golovchenko, Harvard University, Cambridge, MA.

We will discuss the recent realization of an in situ BEEM experiment with epitaxial monolayer of Pb on a 7×7 reconstructed surface of Si(111). The metal film was MBE grown in a UHV chamber and in situ transferred into a room-temperature UHV scanning tunneling microscope modified for three-terminal BEEM measurements. Experiments were performed in a constant-current mode of STM. With the STM tip above the Pb wetting layer increasing the energy of tunneling electrons from 1 to 2 eV yields an abrupt increase of the collector current equal to 10% of the tunneling current. Our experiments show that a Pb wetting layer is a two-dimensional metal separated from the semiconductor substrate by Schottky barrier ~ 1 eV. This feature can be explored for achieving metal contact to a single Pb quantum dot (3D island). Experiments with Pb islands show significant reduction of the collector current versus the wetting layer due to attenuation of electrons with increasing Pb thickness.

11:30 AM P12.11

NUCLEATION AND GROWTH OF TITANIUM SILICIDE ISLANDS ON Si(100) STUDIED BY STM. T.H. McDaniels, J.A. Venables and P.A. Bennett, Dept. of Physics and Astronomy, Arizona State University, Tempe, AZ.

We report an STM study of island nucleation for titanium silicide grown on Si(100) by physical vapor deposition. Island density vs. coverage, flux and temperature are compared with a classical nucleation theory (CNT). The flux dependence at 450C indicates a critical nucleus size of $i = 3$. The temperature dependence in the range 300-700C is well fit by CNT using $i=3$, diffusion energy $E_d = 1.1\text{eV}$ and island binding energy $E_b = 0.4\text{eV}$. These values are not consistent with the direct hopping measurements of Ti-dimer-vacancies ($E_d = 1.8\text{eV}$) reported by Ishiyama et al (Phys. Rev. B51, 1995 p.2380). STM images combined with the scaling behavior for nucleation suggest that silicide formation is dominated by the motion of Si adatoms and a mobile Ti precursor state.

11:45 AM P12.12

DYNAMICS OF ISLAND GROWTH AND ISLAND INTER-ACTIONS OF TiSi_2 ON Si SUBSTRATES. R.J. Nemanich and W. Yang, Dept. of Physics, NC State Univ., Raleigh, NC.

The dynamics of the growth of nanoscale TiSi_2 islands on (001) and (111) Si substrates is explored using in situ, real time UV photo-electron emission microscopy (PEEM). The 50-100nm islands were prepared by in situ deposition of a few monolayers of Ti onto Si substrates. The islands were formed by Ti deposition at room temperature followed by annealing to 1150°C or by continuous Ti deposition onto Si at a temperature of 1150°C. For islands formed by Ti deposition followed by annealing on both (001) and (111) Si substrates, coalescence is observed in which nearby islands apparently "move" directly toward each other and eventually coalesce into a larger island. This process occurs as ripening is observed for other islands. The measured island distribution as a function of annealing temperature indicated that the island density decreases and the average island size increases as the annealing time increases. In contrast, for continuous Ti deposition at 1150°C, the island density does not increase. However, islands grew laterally and vertically, and changed shape. In particular, on the (111) Si substrate, an island shape transition was observed in which the initial circular islands transformed into elongated rectangular shaped islands. Some islands of longer rectangular wire shape grew anisotropically along three equivalent directions. These results are discussed in terms of the kinetics of the different growth processes and the energetics of the different TiSi_2 island structures on the Si substrates.