SYMPOSIUM P

November 27 – December 1, 2000

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*Invited paper
SESSION P1: NANOSCALE SURFACE STRUCTURES
Chair: Franz J. Hengsh
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. Ogule, V.A. Novikov, A.P. Monga, and B. Barnoudi. 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 wafer, which can subsequently be lithographically processed into functional devices. This talk presents 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 NONPLANAR surface features (which we term “TIPS”) by a spontaneous assembly process involving the oxidation of single metal, 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 Pt, 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, nano-electronic devices. S. Aggarwal et al, Science 287, 2325 (2000)

8:45 AM  P1.2
NOVEL AND FLEXIBLE SELF-ORGANIZED ROUTES FOR NANOSCALE PATTERNING, Sebastian van Dijken and Benno Postema, University of Twente, MESA Research Centre and Faculty of Applied Physics, Enschede, THE NETHERLANDS.

The evolution of the morphology of growing Cu(thiol) has been studied in detail using HRLEEM 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 lamellae are formed with step edges along (110). These pyramids assume a checkerboard pattern, with well-established short-range order and weak long-range order. After grating incidence deposition the surface exhibits a distinct two-fold symmetry in contrast to the expected and measured four-fold symmetry at normal incidence. At grating 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 grating 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) on parallel ripples oriented perpendicular to the (110) 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 (112) on the illuminated and the shadow sides of the ripples, respectively. The distance between the ripples is determined by the adsorb mobility. By varying the substrate temperature between about 220 and 350 K their mutual separation changes from about 3 to 15 nm. These 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. Piretich, University of Michigan, Dept of Chemical Engineering, Ann Arbor, MI; David J. Schlozczynski, 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 tangential 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. P.B. Oh, 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 areal 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 striped mode with a disordered surface alloy of 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 380 °C, 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-strips-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 see 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-ACO4-94AL85000.


10:00 AM  P1.5
DYNAMIC STM STUDIES OF THE NUCLEATION AND GROWTH OF SELF-ORGANISED NANOSTRUCTURES. Flemming Bensenbacher, Institute of Physics and Astronomy and Center for Atom-scale Material 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 microscopy can be used to dynamically follow the nucleation and growth of selforganised nanostructures on surfaces. In the first example we have studied the self-assembly of hexasulfur molecules, hexa-tert-butyl decacyano (H6DBC) 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 covered the (110) surface of GaAs(001) with In-oxide nanostructure on Pt(110). Long-range elastic interactions cause this nanostructure to self-organize over mesoscopic length scales into a (11x2) On-monolayer. We will show how this nanostructure can be used as a template to tailor the epitaxial growth metal islands with a narrow size distribution [3].


10:00 AM P1.6
PREFERENTIAL NUCLEATION AND SELF-LIMITING GROWTH OF METAL NANoclUSTERS ON Si(4x4)/W(111). Q. Wu, W. Chen, T. E. Mallouk, Department of Physics and Astronomy and Laboratory for Surface Modification, Rutgers University, Piscataway, NJ.

Interactions of Cu and Pt with the highly ordered Si(4x4)/W(111) surface have been monitored by means of electron spectroscopy for chemical species (AES), low energy electron diffraction (LEED), and scanning tunneling microscopy (STM). The substrate is sulfur-induced nanoscopic reconstruction of W(111) with (4x4) periodicity, characterized by a planar terrace (~20 nm in width). We find that fractional monolayers of vapor-deposited Cu grow as clusters on the Si(4x4) surface over a wide coverage range. At low Cu coverages (< 0.1 ML), Cu nanoclusters are observed to nucleate preferentially at characteristic hollow sites on the Si(4x4) surface; there is a strong 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 Si 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 TDP data.

10:45 AM P1.7
SELF-ORGANIZED NANOSCAPE PATTERN FORMATION ON VICINAL Si(111) SURFACES VIA A TWO-STEP FACETING TRANSITION. P. K. Maj, National Chiang 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. Kwan Kern, Max-Planck-lnstitut 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 nanostuctures are subject to lateral boundary conditions on a length scale which is much smaller than nanoscale objects. Magnetic nanostuctures can be made out of traditionally nonmagnetic elements, and 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 nanostuctures 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 nanostuctures 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 nanostuctures will be presented. By way of illustration the growth of one- and two-dimensional arrays of metal nanostuctures, luminescent Ga quantum dots and supermolecular nanographites will be discussed in detail.

11:30 AM P1.9
TAILORING THE SIZE AND SHAPE OF METALLIC NANO-structures THROUGH LASER IRRADIATION DURING AND AFTER GROWTH. Frank Stiefl, Johannes Beulbach, Thomsa Wenzel, Frank Trüger, 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 these 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 nanoparticles occurs, making it difficult to control both parameters almost impossible. Here we show that laser irradiation of metallic nanoclusters 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 nanoclusters 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 monodisperse samples. The methods are demonstrated experimentally for Ag and Au particles with diameters between 1 and 25 nm using different oxide surfaces including Si 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 nanoparticles quantitatively.

SESSION P2: PATTERN FORMATION ON SURFACES
Chair: Michael S. Altmann
Monday Afternoon, November 27, 2000
Room 302 (Hyenas)

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 essence physical process concerns the island shape transition in 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]


2:00 PM P2.2
NANOSCAPE PATTERN FORMATION OF AN EPITAXIAL MONOLAYER GROWN ON A SOLID SURFACE. W. Liu and Z. Yan, 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 selforganize into superlattices. This paper reports on a simulation of the pattern formation process. We show that the size selection and selforganization 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/~matm.
Self-assembled superstructures of gold nanoparticles are studied using high resolution TEM and high dispersion diffraction methods. The optimal object for observation of such structures is described. The size and the crystallization condition is possible to produce different crystaline structures such as cubic or hexagonal close packing or tetragonally distorted fcc. The coating method which is selected is discussed. The evolution of the superstructure of the self-assembled superparticles is also reported. The experiments were carried out in situ heating in the high resolution TEM. The temperatures were varied until reaching the melting point of the superstructure. The melting mechanism is discussed.

6:00 PM P2.2
SELF-ORGANIZED ARRAYS OF DOTS AND STRIPES AT STEPPED SURFACES. Franz J. Himpsel, Univ Wisconsin Madison, Dept of Physics, Madison, WI.

Self-organized nanostructures are ideal testbeds 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 microstructural studies are 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].

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 makes either stripes or strings of dots. A new growth technique for gold on stepped Si(111) faces is proposed [2].

2. Selective adsorption of molecules between calcium fluoride stripes and its extension to selective CVD of iron nanowires. Organic molecular and DNA nanogaps on stepped silicon structures that are made biocompatible via thiol-gold chemistry. One-dimensional chains of gold on stepped Si(111) with exotic band structures [3].


6:30 PM P2.3
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 heterogeneous substrates, and can typically be described in terms of three energy parameters. A few cases of nucleation on substrates containing defects have been investigated, at the cost of introducing (at least two) more parameters. Growth methods using patterned substrates and for 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.

6:45 PM P2.4
DYNAMICS OF InAs QUANTUM DOTS FORMATION ON AlAs AND GaAs. M. Yakimov, V. Tokmanov, and S. Oskolkov, Center for Advanced Thin Film Technology, University of Alabama - SUNY, Albany, NY.

We have studied the formation of InAs quantum dots (QDs) grown by molecular beam epitaxy on top of GaAs and 2 μm-thick AlAs overlayers in a temperature range from 480°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 and 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 dependence of sizes and shapes of the QD ensemble. The critical angle for QD formation was shown to be 1.5° higher (at 400°C) for dots grown on the AlAs overlayers that 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 which exhibits a distinct minimum at 450°C if grown on AlAs overlayers. The increase of the critical coverage with temperature reduction is attributed to the lower surface diffusion rates of adatoms on the AlAs surface.

4:00 PM P2.7
SELF-ORGANIZED COARSENING OF TWO-DIMENSIONAL ISLANDS VIA STRAIN-DIRECTED ISLAND MOTION. Feng Lin, Anh H. Li, and M.G. Lagally, University of Wisconsin, Dept of M&SE, Madison, WI.

We show that in coarsening of two-dimensional islands, 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 islands with uniform size and spacing.

4:15 PM P2.8
PERIODICAL DISLOCATIONS NETWORKS OF Ge FILMS ON Si(111). Th. Schmidt, J. Falta, Univ Bremen, Bremen, GERMANY; P. Zübl, M. Krämer, P. Kury, Univ Hanover, Hanover, GERMANY; M. Horn-von Hoegen, Univ Essen, Essen, GERMANY.

Thin Ge films grown on Si(111) have been investigated by spot profile analysis of low energy electron diffraction (LEED) and grazing incidence X-ray diffraction (GIXRD). At a substrate temperature of about 700°C, Ge films were grown by standard surface 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(110) 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 mild 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 periodic 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 5 Å thickness is about 1.0% and decreases with increasing film thickness. From an analysis of the width and the relative 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
SPECKLED LIGHT ON SURFACE REACTIONS. IMAGING PATTERN FORMATION FROM ULTRA-HIGH VACUUM UP TO HIGH Pressures. Harm Hinrich Roesmann, 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 Ellipsometer Microscopy for Surface Imaging (EMSI), based on an ellipsometric effect, and Reflection Anisotropy Microscopy (RAM) using different reflectivity properties of non-magnetic surfaces, extend 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 reations. An advanced version of the RAM using just white light in combination with a custom-designed Fourier-transform 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.

This is a richly illustrated talk and ends with a discussion.
P3.1 SURFACE SELF-DIFFUSION INSTABILITY IN ELECTRIC FIELDS. Michael L. Ogden, Pawel P. Palczewski. Scientific and Industrial Association “Hitex”, 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 where 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) electric 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 the surface the stronger is the intensity of near-surface electrical field. Consequently two competing effects of self-diffusion: 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 length below 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 between molecule and the electric field. Thus the stronger 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 atoms 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. Baryshnikov, 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 special interest because it was investigated experimentally well enough, for example, by electron and neutron scattering on such structures in 3D crystal. 1D adatom structures can be formed on the anisotropic substrates. In atoms on the W substrate and atoms of inert gases 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 dispersion 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, which due to 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 GROWING AND MIGRATION OF INCLUSION/GROOVE BOUNDARIES. Harriet W. Young, Harrison Weng. 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 growing has not been studied in detail. We have coupled thermal growing and grain-boundary migration for slightly inclined grain boundaries, and obtained free-surface and grain-boundary profiles. We assume that thermal growing occurs in a 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 CHEMOSORPTION AND DIFFUSION OF OXYGEN AT DEFECTED Al[111] SURFACES. Naboni Rashid, University of Virginia, Dept of Material Science and Engineering, Charlottesville, VA; M. Neurock, University of Virginia, Dept of Chemical Engineering, Charlottesville, VA; H.N.G. Walker, University of Virginia, Dept of Material Science and Engineering, Charlottesville, 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 eV) 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 23 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 Minyayev, Nikolai Tsvetov, Irina Nosulenko, Rostov State University, Dept of Physics, Rostov on Don, RUSSIA.

The shape of small liquid inclusions enclosed in a miniscopic solid changes under the action of weak (< 10) 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 CdTe photovoltaic cells. The 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 critical 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 material 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 ION BEAM ASSISTED DEPOSITION. Jussi Silhanpää, Accelerator Laboratory, University of Helsinki, Helsinki, FINLAND; Iivo 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 computer simulations to gauge the relative importance of different atomic processes in promoting layer-by-layer growth.

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P3.8
CALCULATION OF THE DIFFUSION COEFFICIENT OF EQUILIBRIUM SYSTEMS WITH ATTRACTIVE INTERACTIONS.
Eleon Arapaki, Pras Aragakis, Department of Physics, University of Thessaloniki, Thessaloniki, GREECE; Michael C. Trinigk, 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 annealed to a fixed temperature T, it evolves in time from an initial random state to attain the [111] 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 constant of the autocorrelation function for various temperatures of the system, ranging from 0.8Tc to 0.95Tc. It is possible to reduce 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.
Michiel H. Haefel, Naval Research Laboratory, Washington, DC; and Olivier P.-L. UijR, 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 "rackets". An external AC driving force can lead to mound formation, or flatten the surface. Using a general formulation based on the Burton-Cabrera-Frank (BCF) model, we describe the AC driving of a surface with temperature, an electric field, or an elastic strain, and calculate the AC driving force leading to morphological changes. The basis of the kinetic Monte Carlo (KMC) simulations, the variation of roughening and island coarsening exponents with temperature and frequency are calculated. As a quantitative example, we consider AC variations in electrochemical potential. Using surface embedded atom method potential 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 nonstationary 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 model for the calculation of strain effects in lattice mismatched systems. This approach allows us to self consistently calculate quantities like the strain-energy density for a given surface configuration at any given point by only the elastic constants of the involved materials and the boundary conditions. In this model, step velocities are determined from the equilibrium adhesion 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 is due to a logarithmic attraction of steps that 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 experiments of Tersoff et al., the height of the bunching of the epilayers is observed to be dependent on the elastic constants of the underlying substrate plays a crucial role for the evolution of the epilayer surface.


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 for II-VI semiconductors. The model includes 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 and our analytic model experiments agree with 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. Jin-Wook Lee, Jeongyong Lee, Korea Advanced Institute of Science and Technology, Daejeon, KOREA.

Atomic migration at highly 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], [112] 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 lining 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. Karl Wiesinger and Gunther Springholz, Johannes Kepler Universitat, Linz, AUSTRIA.

The formation of growth spirals on the surface of epitaxial layers is a widespread phenomenon in lattice-mismatched heteroepitaxy which has been observed for a large variety of material systems, ranging from high Tc 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 mono-lamellar heteroepitaxy 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 α = 1 as compared to α = 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 incoherent layer growth mode. This strong deviation is due to the strong coupling of the surface step motion by adatom surfice diffusion for high growth rates. 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.


P3.14
BOUNDARY CONDITIONS FOR ADATOM DIFFUSION IN EPITAXIAL GROWTH. Russell Callisch 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 adatoms/and ions 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 Gibb's-Thomson films 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 results from using a reactive segregation equilibrium model and from kinetic Monte Carlo simulations.

P.3.15
EVOLUTION OF SURFACE STRESS DURING GROWTH OF GOBALT 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 silicon islands by reactive deposition. Island structures (coverage, aspect ratio, and coalescence) are determined ex situ using TEM and AFM (Fig. P.11) at T = 600° C. We observe a surface stress of \( \sigma = 0.5 \pm 0.1 \text{N/m} \) and a metastable phase with Inset mismatch of 0.5%. For \( T = 800° C \), Inset varies through several cycles of compressive/tensile stress in the coverage range 0-20%. This is attributed to a sequence of silicon phases and coverage. On Si(100), the stress is \( 0.06 \pm 0.05 \text{N/m} \) for all T in the range 25 - 800° C. This low value of stress is attributed to a mixed orientation of CoSi sub2, which is expected to be independent of growth temperature.

P.3.16
DEVELOPMENT OF EXTREMELY HIGH LEVELS OF STRESS DURING DEPOSITION OF FULLERENE-LIKE C60 THIN FILMS BY UN-BALANCED MAGNETRON SPUTTERING WITH LOW ION ENERGY BOMBARDMENT. Jan Brunell, Jürg Neidhardt, Zach Czigány, Lars Holmström, 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 stress in the recently discovered flexible fullerene-like C60 thin films and the effects of deposition parameters on stress development. We investigated the effect of deposition parameters on stress development of C60 thin films in a situ during growth. Thin films \( \approx 500 \text{ nm} \) thick were deposited by unbalanced, reactive magnetron sputtering in an Ar/N2O atmosphere. The radius of curvature was enhanced in situ 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 microstructure was investigated by SEM, the deposition by AES, and the mechanical response to a meandertest was recorded. The stress was observed to be initially tensile, then, after \( \approx 20 \text{ min} \), it becomes compressive, reaching a maximum of as much as \( 7 \text{ GPa} \), 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, \( \approx 20 \text{ eV} \), and such low ion-to-neutral arrival rate ratio (typically \( < 0.1 \)). In conclusion, deposition of pure carbon films under similar conditions yielded much lower stress levels, typically \( \approx 1 \text{ GPa} \). We believe this effect is related to the lack of oxygen from the deposition atmosphere, which results in the high oxygen content of the films.

P.3.17
MOLECULAR-DYNAMICS STUDIES OF VOID GROWTH IN STRAINED DUCTILE METALLIC THIN FILMS. M. Roaf Gungor and P. Oehrle, 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, dipoles, and larger scale defects such as voids. In this study, we present the results of molecular dynamics simulations performed in the preparation of thin films using a set of atomistic simulations. 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 interconnects in integrated circuits. In our atomistic simulations, the interatomic interactions are described by an embedded-atom method (EAM) parameterization for copper. Molecular-dynamics (MD) simulations are carried out using large, multi-nanometer 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 thin films is found to occur through void growth mediated by plastic deformation and self-diffusion mechanisms. Dislocation emission from the surface of voids into adjacent voids and subsequent propagation through the film are demonstrated as primary mechanisms that reduce residual stress. Void growth and stress reduce in the film are analyzed in detail. In addition, mechanisms of mechanical 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 softening mechanism that may be involved in devices at interfaces between the metal and thick-film materials due to intergranular stress relaxation. The results of the present work are compared with previously reported experiments. The results of the present work are compared with previously reported experiments. The results of our kinetic analysis are incorporated into continuum-scale self-consistent dynamical models of mechanically-induced thin-film failure. Implications of the present model for applications in high-performance electronic devices are discussed.

P.3.18
MICROSTRUCTURE EVOLUTION IN THIN FILM AND NEAR SURFACES PHASE FIELD MICROELASTICITY APPROACH. Yongmei M. Jin, Arneun 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 Phsce Field formalism, this solution provides the computational model that is as efficient as the existing PFM model for the bulk system. This modified theory makes it possible to realistically simulate the 3-D evolution of the coherent multidomain and morphotropic microstructural defects as well as inhomogeneous 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 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 influence 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.

P.3.19
IN SITU STUDY OF TITANIUM FILM GROWTH ON DIFFERENT SUBSTRATE SURFACES. Paul Oehrle and Reinhard Abermann, Univ. of Innsbruck, Inst of Physical Chemistry, AUSTRIA.
The growth of thin Ti-films on different substrate surfaces was investigated under UV-conditions by in situ stress measurements. The main objective of these measurements 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 TiO2 film prepared by reactive evaporation of Ti in an oxygen atmosphere and post-annealing. The Ti2O3 growth on this substrate is compressive up to monolayer coverage and tensile at higher film thickness, which is indicated to be an effect of the interface between the TiO2 film and the metal substrate. The Ti2O3 growth on this substrate is compressive up to monolayer coverage and tensile at higher film thickness, which is indicated to be an effect of the interface between the TiO2 film and the metal substrate. In a second series of experiments the TiO2 film was covered with Al-overlayers of increasing thickness. Due to oxygen interdiffusion from the TiO2 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 monolayer of Al gives 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 is observed 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 determined from the changes in the tensile stress will be compared with that seen on Al-Microstructures. (ii) A tensile stress contribution (with an incremental stress up to 4 GPa) is attributed to alloy formation. Osmot and magnitude of this latter tensile stress depend on the Al-film thickness and substrate temperature during Ti-deposition. Phaseview TEM-micrographs and TED-results will be shown. For comparison, analogous experiments were made with AlOx and Al2O3 layers. The results of these experiments qualitatively agree with those on the TiO2/Al substrate.

P.3.20
IN SITU INVESTIGATION OF TiAl 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-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 underlying AlN film prepared by reactive evaporation of Al in an oxygen atmosphere - was used. The substrate temperature (T_s) was varied from room temperature to 800°C and the AlN thickness from Ti to Ti/Al. At T_s = 500°C the film stress is compressive and the dependence on stoichiometry is rather small. Only the stress vs. thickness curve of TiAl films shows unexpected oscillations during growth while at lower aluminium content the stress shows stress curves are measured. The stress changes after deposition are large in each case, interpreted to indicate film recrystallisation. While the TiAl phase was identified by XRD results a positive identification of the TiAl phase was not possible. In a further series of experiments the growth stress of TiAl films was investigated at 100°C < T_s < 400°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 stress-stoichiometry was investigated at T_s = 300°C. At low film thickness the stress vs. thickness curves are similar, however, at film thicknesses above 800 nm they differ significantly and show either tensile or compressive stress changes (1500/µm) stresses in 1500 nm 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.

P.3.21
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 strain affect the activation barrier for adatom migration. A change in diffusion coefficient may then be related to the change in the activation barrier.

P.3.22
ATOMICISTIC MODELS FOR THE SURFACE STRESS OF FCC METALS WITH APPLICATION TO SURFACE RECONSTRUCTION. Toms T.M. Tribble and R.C. Cammisa, 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 unreconstructed surfaces, and by computer simulation for fully relaxed surfaces. Pair-potentials are inherently unable to describe real metal surfaces 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 (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 the adhesion strain and fracture strength as a function of the fracture surface can be well reproduced by computer simulations using the analytic EAM potential, and it is also in good agreement with a simple continuum thermodynamic model involving the surface stress, surface free energy, shear modulus, and lattice parameter.

P.3.23
DETERMINATION OF g-FACTOR VALUES OF ULTRATHIN FILMS OF Fe/InAs(100) BY BRILLIANCE LIGHT SCATTERING. Guang-Xu Geng and Hong-Ru Zhu, Laboratory of Solid State Microstructures and Center of Materials Analysis, Nanning University, Nanning, CHINA; Ya Zhang, Dept of Physics, South East University, Nanjing, Jingshui, CHINA; Y.H. Xu, E.T. F. Remoissenin and J.A.C. Bland, Cavendish Laboratory, University of Cambridge, Cambridge, UNITED KINGDOM; Jin 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 observation. A dominant and in-plane producible fourfold magnetic anisotropy was clearly present in Fe(100)ML films from the magnetic resonance (MR) frequency (GHz) versus orientation angle (degree) of the in-plane applied magnetic field. When the thickness of Fe layer is decreased the in-plane magnetic anisotropy is suppressed. 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 are given. Reference: [1] Y.B. Xu et al., "Applied Physics Letter" 73 (3) 333-340 (1998).

P.3.24
MECHANICAL AND RESISTANCE MEASUREMENTS ON BORON-DOPED AND UNDOPED NiAl THIN FILMS. Edward Pettersson, Lawrence L. Henry, Southern University and A&M College, Baton Rouge, LA.

We report preliminary results of magnetization and IV measurements of the effects of boron doping on the magnetic and electron transport properties of NiAl 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, the temperature is increased through the transition range dM/dT fluctuations between negative and positive values, and the magnetization changes from positive to negative near T = 52 K. Results of four probe IV 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 5 T) 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 \cdot 230 K temperature range. This transition is not seen in the doped sample.

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P.3.25
CRYSTAL STRUCTURES OF Mn AND Fe THIN FILMS GROWN ON GaAs (100) SUBSTRATES DETERMINED BY SYNCHROTRON RADIATION DIFFRACTION. Y.Z. Wu, D. Qin, W.X. Tang, D. Wu, G.S. Dong and X.F. Jin, Surface Physics Laboratory, Fudan University, Shanghai, CHINA; Q.J. Jin and X.M. Jing, 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 techniques 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 results 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 400 K have a face-centered-cubic-like structure. The in-plane lattice constant of Mn films determined by grazing angle incidence x-ray diffraction is a = 3.8212 nm, and the out-plane lattice constant determined by large angle incident X-ray diffraction is c = 3.9728 nm. The ratio of a to c is about 1.00. This indicates that the in-plane 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 = 2.8262 nm (in-plane) and c = 2.9808 nm (out-plane) respectively. The ratio of a to c is about 0.95. The structure of Fe thin film on GaAs (001) is close to a hcp structure.
Besides, the standing wave configurations also are clearly observed in the X-ray diffraction intensity profiles from Fe thin films, which implies that the film thickness is small enough to have a nearly smooth layer. The atomic layer spacing in the direction perpendicular to the surface of Fe thin films derived from the nodal position of the X-ray standing wave is 0.145nm, 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. Shangguang Liu, Naijuan Wu, Alex Ignatiev, Space Vacuum Epitaxy and Center Texas for Superconductivity, University of Houston, Houston, Texas, US.

Cobalt Magnetoresistive (CMR) thin films have shown a large electric-pulse-induced resistivity (EPIR) change effect in zero magnetic field. One of the main temperature dependences of these films can be both decreased and increased through multiple nonvolatile intermediate levels by short electric pulses. An enhancement of this effect has been seen for Pr0.6Ca0.4MnO3 (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 pulsed annealing were subjected to 170°C in air for 0.5 hr. Upon cooling the films showed increased in the nonvolatile resistance ratio ΔR/Rmin = (Rmax - Rmin)/Rmin by more than 700%.

P3.27
MAGNETIC THIN FILMS PREPARED BY SOL- Gel PROCESS. Luciano Scorn, Nely Della Statina Mohol, Federal University of Minas Gerais, Dept of Chemistry, Belo Horizonte, BRAZIL.

Nanostructured particles have been researched due to their high surface/volume ratio, 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 ferrite dispersed in a silica matrix were prepared by sol-gel process using metallic nitrates as a precursor of the ferrite and tetramethylorthosilicate (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 porosity parameters such as ferrite concentration, dipping velocity, solution viscosity and heat treatment temperature were correlated and associated with the coating morphology and magnetic properties. The composition of the films was determined by X-ray fluorescence using synchrotron radiation. The morphological properties were analyzed by atomic force microscopy and the magnetic behavior by magnetic force microscopy. Porosity and refinement index were estimated by spectroscopy UV/visible.

P3.28
PERPENDICULAR MAGNETIC ANISOTROPY IN ULTRATHIN YIG FILMS PREPARED BY PULSED LASER DEPOSITION TECHNIQUE. Eugeign. Brogoin, Nils Koller, Marcel Gugel, Mark-Clare Bienecke, Michel Tesser, 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 hcp, 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 - 300 K. Ferromagnetic resonance (FMR) studies of samples with thickness 100 - 3000 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 (4πMeff/J) approximately allowing 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 with the thickness-dependent effective magnetization for a given temperature decreased with decreasing sample thickness. This can be caused by an increasing contribution of the surface anisotropy to 4πMeff when the sample thickness is reduced.

P3.29
EFFICIENT GROWTH OF (001) AND (111) Ni FILMS ON MgO SUBSTRATES B.A. Lekanov, Y.A. Stoinic, C. Uher and R. Clarke, Physics Department, University of Michigan, Ann Arbor, MI, USA.

Metal-ceramic interfaces are important applications in 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 annealing conditions so that other physical properties can be tailored for specific applications. We will present our studies on the epitaxial growth and annealing of (001) and (111) Ni films 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. Bogliini, G.J. Clarke, J.F. Ziegler, Nucl. Instrum. Meth. 218 (1983) 445.

P3.30
DEPOSITION-ORDER-DEPENDENT MAGNETIC PROPERTIES OF CoNi/Gd BILAYERS. B. Altenbuchner and A.R. Keyser, Department of Physics, University of Texas at Arlington, Arlington, Texas, US.

CoNi films were grown on thin Gd substrates 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 depended 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. Aign, H. Srikant, 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. Xiono, 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 CrO2 films. The thin films grown epitaxially on (100) TiO2 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 for the full angular dependence of transverse susceptibility. Work at ARO is supported by the US Department of Defense through DARPA grant No. MDA972-95-1-033.

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, USA.

 Giant magnetoresistance observed in cobalt-copper multilayer films prompted 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 useful 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 magnetostriiction. DC magnetron sputtered [Co/Cu] multilayer films were prepared in a sputtering chamber with an in-situ stress measurement system. The first few monolayers of Co show a tensile stress consistent of 4.5 GPa, roughly consistent with expected coherency stresses associated with the lattice mismatch. For greater Co thickness, the stress decreases but remains tensile. Copper layers show an initial compressive stress of ~ -2.5 GPa, lower than that expected from coherency stresses. Continued Cu growth results in a reduced compressive stress. For a [Co 3 A // Cu 21 A] film, with 20 bilayers, the total film stress was approximately tensile, with the largest magnitude in the Co layer far from the device manufacture. Additionally, films grown with In surfactant layers show different stress behavior, implying that the surfactant layer changes the surface energy and film microstructure. The roughness and intermixing of films 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 lead to a more complete understanding of growth processes and control.

P.3.35

STRUCTURAL AND MECHANICAL PROPERTIES OF AMORPHOUS Zn-BASED ALLOY THIN FILMS. S. G. Mayr,1
Physikalisches Institut, Universität Göttingen, Göttingen, GERMANY; M. Moske, Forschungszentrum Jülich, Borm, GERMANY; K. Samwer,1 Physikalisches Institut, Universität Göttingen, Göttingen, GERMANY.

The evolution of surface structures of coevaporated and sputtered amorphous ZnGaAs, AsGa, and CuGaAs films with varying deposition conditions is investigated. The in situ deposition of thin films reveals pronounced structure formation, depending on parameters, such as substrate temperature, film composition (variation of the Zn content) and the angle of incidence, compatible 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]. Presumably these atomic processes, it is possible to model the evolution of the structures of amorphous thin film growth by the use of stochastic continuum growth equations, which are numerically solved [2]. Additionally, the connection to intrinsic stress formation during film growth is discussed.


P.3.34

ELECTROMIGRATION-INDUCED SURFACE WAVE PROPAGATION ONVOIDS IN METALLIC THIN FILMS. M. Hailg and K. Samwer, Dept. of Chemical Engineering, University of California, Santa Barbara, CA.

Failure of metallic thin film interconnects is among the most important problems of reliability issues 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 energy is computed in a computer program with the anisotropic 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 and form periodic surface waves. Both of these types of void waves 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 to predict the onset of failure following surface wave propagation is derived.

P.3.35

THE EFFECT OF Pb ON THE INTERFACE STRUCTURE OF Fe/Cr(100) METALLIC MULTILAYERS. Miso Kimikita, Kyo-Young Kim, Sing-Man 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 interface. Numerous observations have been reported, indicating that interface roughness plays a key 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 roughness and electrical property in metallic multilayers, we have fabricated Fe/Cr(100) multilayers with and without surfactant by molecular beam epitaxy. We investigated the differences in the interface structures and magnetoresistance 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 those 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 is 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 magnetoresistance property of Fe/Cr(100) multilayers.

P.3.36

ELECTRONIC STRUCTURE OF Ag/Cu(111) DOUBLE NANOFLM STRUCTURES STUDIED BY ANGLE-RESOLVED PHOTOEMISSION SPECTROSCOPY. Akio Tsuchik, Inst. of Science and Technology, Osaka University, Japan; Hiroyuki Kitahara, Tohoku University, 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 structure 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. The electronic coupling between the quantized states is one of the situations that differ from 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 the magnitudes of the coupling 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 is 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 layer 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.

P.3.37

PULSED LASER DEPOSITED NANO CRYSTALLINE ZnO THIN FILMS. Raj K. Thang, Kumamoto University, Japan; Anil Chandra Mook, Institute of Technology Kharagpur, INDIA.

In recent years, there has been a great interest in wide-gap materials because of their potential applications in optoelectronics and electronics. One of the problems that has plagued the development of GaN has been the lack of high quality, closely lattice matched materials. Recent work has shown that ZnO thin films are being grown on sapphire substrates by pulsed laser deposition, resulting in a light emitting diodes. 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 this work, we report on the pulsed laser deposition of ZnO at room temperature (RT). The deposition was done on silicon and glass substrata at RT under the oxygen pressure ranging from 10 mTorr to 1 Torr. We used a frequency tripled third-harmonic (355 nm, pulse width of 10 ns) at 10 Hz from an 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 [001] plane. The grain size calculated using Scherrer's formula decreases as the oxygen gas pressure decreases. 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 [3.12 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 355 nm radiation. The pump beam was focussed onto the sample face and the emission was collected by 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. Edelot, L.B. Kish, E. Coccoz, O. Olsson, and C.G. Granqvist, Department of Physics, 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 723 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 723 K. Scanning Electron Microscopy was applied to two of the samples, one with high density and one with low density, to analyze 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. Chonguang, J. Edelot, 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, Linkoping, SWEDEN.

In-situ electrical transport measurements were carried out in nanocrystalline gold films during inert gas deposition. The time dependence of the conductivity showed self-organization phenomena, including aspects of: i) biased percolation; ii) conductor-insulator transition; iii) biased percolation; and iv) conductor-good conductor transition, - annealing, sintering, - electron microscopy. The different effects were identified by reversing 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 VINCIAL GALLIUM ARSENIDE PLANE. Aksel Sirenkin, Aleksandr Bagasov, Vladimir Makeev, Inst of Radio Engineering and Electronics of NAS, 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 non-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 and method of angular constraints imposition on images of irregular shapes were used. For 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 the surface. It was determined, that the initial vicinal plane before delta-deposition, it was shown that more than 70% of Sn atoms may be in the chain body, and the others 30% has uniform distribution on the terraces of the vicinal plane.


P3.41
FRACTAL CHARACTERIZATION OF THE MORPHOLOGY OF CLUSTER-ASSEMBLED CARBON FILMS: Claudio Castelfranco, INFN - University of Milano-Bicocca, Dept. of Physics, Dept. of Materials Science, Milano, ITALY; Alessandro Posta & INFN - Universita' di Milano-Bicocca, Dept. of Materials Science, Milano, ITALY; Paolo Pineri, Emanuele Barborini, Paolo Milan, INFN - Universita' di Milano, Dept. of Physics, Milano, ITALY.

The morphology of nanocrystalline materials affects most of their physical and chemical properties. Cluster assembling of thin films has recently emerged as the key mechanism for the growth of nanosystems having a structure at the nanoscale. The ability to control the morphology of non-crystalline 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 nanocrystalline films grown by Supersonic Cluster Beam Deposition. We have investigated the dependence of film morphology on different cluster size. After deposition on a Si substrate, the films are uniform and flat. At higher thickness, roughness increases and dessorbed isolated structures, much larger than the basic units, appear. Above a characteristic thickness, depending 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. Semkow, Lynne A. Samselson, Il-Yong Kim, Materials Science Form, U.S. Army Natick Soldier Center, Natick, MA; Changmoo Sung, Center for Advanced Materials, University of Massachusetts, Lowell, MA.

Crystalline and amorphous aluminosilicate particles were obtained at temperatures between 300°C and 50°C through the mineralization of aluminum oxides and silicon oxides onto multilayer polymer film templates. Crystal structure, phase identification, and morphology were determined 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 powders were determined. 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 SiAlO 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.H. Kennedy, M.J. Brett, Dept. of Electrical and Computer Engineering, University of Alberta, Edmonton, Alberta, CANADA; T. Pate, 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 isotropic 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-shaping mechanism in three dimensions. Apart from this academic motivation, there is the need to characterize the physical, mechanical, porosity, and scalability of these systems. In this study, we will test the hypothesis for the realization of isolated, periodically arranged nanostructures envisioned for a class of applications. Results from an ongoing study of growth dynamics, morphology, porosity, and scalability will be presented. The opportunity 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-FLM.

P3.44 Abstract Withdrawn.

P3.45 GROWTH MORPHOLOGIES AND SURFACE ENHANCED RAMAN SCATTERING OF PLATED SILVER ON NANO-PARTICLE 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 with long wavelength scale were all observed and shown 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 parametronic silver excited with gold-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 HOMOEPIXY OF GAs ON (100) AND (100)/(111)A SURFACES. M.A. Nemirovskaya, R. Venkatraman, 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 most frequently used, 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 homoeopxy of GaAs under VPE conditions and the evolution of the (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-sustaining effects for microstructure predictions on this surface. Also, we observe directly the evolution of the (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 in the investigation of the deposition on complex patterned surfaces.

P3.47 MICROSTRUCTURE AND OPTICAL PROPERTIES OF C-SiPUMER DEPOSITED Si:Al NANOCOMPOSITE THIN FILMS. Peng Niu, Department of Materials Science and Engineering and Materials Research Center, Northwestern University, Evanston, IL; Peter J. Balsara, Brian Harper, 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, photoconductive and thermionic emitters, due to enhanced surface plasma resonance absorption mode of nanosized 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 spectroscopy in the wavelength range from 200 to 3000 nm. Film microstructure was found to consist of nanosized Al particles (<10 nm) embedded in an amorphous SiAl matrix. The optical absorption spectra of the films up to 50 at. % Al exhibited a sharp increase, which is related to the 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, absorption peaks were between 300 and 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 TRANSLATIONAL MOTIONS OF MICROSTRUCTURES FORMED DURING CRYSTALLIZATION OF THIN AMORPHOUS FILMS. Vladimir Yu. Kolesov, 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°] perpendiculate distortion of the surface is present around an axis (or axes) lying in the film plane. This internal lattice bending (transcrystallization microstructure) has been revealed and studied [mostly in situ, using transmission electron microscopy, constant curvature technique [3]] for the films of different chemical bonding, prepared and stabilized by various methods: Sn, Pb, S, Sb, Ge, SiO, Ni, Cu, Sn, Ge, Te, Fe, O, Co and others. In some cases the present paper we describe geometry, morphology, texture, gradients of lattice orientation, dynamics of crystal growth for the different kind 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 height 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. Kolesov, Proc XII CEM. Settle, 1, 574 (1990). [2] V.Yu. Kolesov, A.R. Tillen, Acta Met., 48, 1829 (2000).

P3.49 Abstract Withdrawn.

P3.50 MESOSCOPIC PATTERNING INDUCED BY CO-DEPOSITION OF C60 AND Ni ON THE MgO(100) SINGLE CRYSTAL. Jan Vrecka, Hiroshi Niiro, Kuma Nakano, 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.

Sporadic generation of complex ordered structures in inorganic systems is both arresting and potentially useful. It is apparent from single compounds, composites and alloys as well, and takes place in various spatiotemporal scales. Here we describe the self-arranged mesoscopic stripe structures formed during co-deposition of C60 and Ni on the MgO(100) substrate. It was found that the periodic stripe systems could be grown if specific deposition kinetics (e.g. deposition rates of C60 and Ni < 0.1 nm/s, temperature of substrate ~300°C, thickness of the Ni C60 adlayer ~100 nm) is applied. Several hierarchically grown self-organized assemblies were observed in the system. The assemblies comprised hundreds of micrometers long domains with thickness and spacing of 1-2 μm and height of about 1 μm. The stripes are oriented into a thin platform consisting of epitaxially grown Ni and C60 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 C60 film, and C60/C60 micromesh clusters is suggested. The periodic stripe system observed in the Ni C60/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 Han, Junichi Mitochi, Takeshi Fukui, Research Center for Interface Quantum Electronic, 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 SiNx masked GaAs (100) substrate. The mask layers were patterned to lines across the [110] direction and were covered by a Ni layer. The rectangular openings attached to the lines. As a result of SA-growth pyramidial shaped GaAs structures were constructed at the rectangular regions of the pattern. A very narrow (110)-facet, in the range of 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 SAQDs on narrow (001)- facets. The design parameters of the patterns such as mask opening ratio, adatom sink around pattern definition also affect the SAQDs formation. The number of the SAQDs formed on the (001)-facets 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 approximated by low temperature spatially resolved photo-luminescence (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. Fans, Shigeru Niki, Hiroaki Okugami, 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 had in the substrate surface plane and parallel to the substrate [110] direction, while the [001] axis of the film was found to be predominantly in directions at 7.5 degrees from the substrate surface normal. The tilt axes were oriented approximately parallel to the [100] and [110] 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 lattice 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, or partially, the film must be rotated by 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 Cretegny, 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 simple model. In continuous 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 etch 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: Ben Hynes
Tuesday Morning, November 28, 2000
Room 302 (Hynes)

8:30 AM P4.1
UNUSUAL MAGNETIC PROPERTIES OF Fe/Ni BILAYERS ON Cu(100).
Xingfeng Liu, Bernd Schirmer, Matthias Wuest, RWTH, Aachen, GERMANY

The epitaxial growth of 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 at the Fe/Ni interface, and a strong influence of the Fe film thickness on the magnetic properties of the Fe/Ni multilayer is found. This leads to an unusual magnetic ordering at the Fe film surface. The magnetic coupling does not only depend upon the Fe film thickness and temperature, but also on the Ni film thickness. This behaviour is correlated with the film microstructure 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. Altmin, 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 recent work to gain control of this 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 (SLEEM) investigations will be described that reveal a new relationship between growth properties, microstructure and magnetism in Fe/Cu(100). By monitoring diffraction intensity oscillations and the evolution of magnetic domains simultaneously and continuously during growth with SLEEM, 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 low energy electron diffraction (LEED) and SLEEM 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
RELATION OF THE ELASTIC STRAIN OF Fe-Pd GROWN ON Pd(100) AND Fe-Pt GROWN ON Pt(300), THIN FILMS
D. Halley, A. Merry, Y. Samson, J.P. Attire, P. By, DFRMC/SP2M/NL, 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 layered consisting of a combination of metals, oxides, or alloys. Nevertheless, ordered magnetic alloys grown by molecular beam epitaxy (Co/Pt; Fe/Pd, Fe/Pt...) 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 thickness of the epilayer with respect to the substrate, relaxation defects may appear and affect the magnetic properties. In the present work, we have investigated the magnetic strain of Fe-Pd and Fe-Pt grown on Pd(100) and Pt(300), using transmission electron microscopy that the relaxation occurs mainly by the formation of microtwins. These twins are formed by the successive gliding of partial dislocations of Burger's vector 1/4,1,1,2 on the inclined planes (111). These defects lead to the formation of defects at the surface of the epitaxial layer. n/2 (in lattice units), aligned along the [110] in-plane directions and the number of partials 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 can be interpreted in the framework of an elastic model of the relaxation. Then, the interplay between microtwins and magnetic properties will be presented.
MESOSCOPIC MAGNETS, DOTS, WIRES, AND PILLARS ON THE NANOSCALE.
J. Kirschner, Max-Planck-Institut für Mikrostrukturphysik, Halle, GERMANY.

Mesoscopic magnetic structures play an increasingly important role in magnetic storage technology, magnetic sensors, nonvolatile 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 and adsorbed inorganic nanoparticle growth phenomena, and self-organization will be exploited to produce and characterize mesoscopic magnetic structures. For example, magnetic wires may be made by step growth in single-crystal surfaces by 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 are formed. 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. Rezaei Pournaz|, Matthias Schefler, Fritz-Haber Institut der MPG, Berlin, GERMANY; Kristen Fichthorn, Department of Chemical Engineering, Pennsylvania State University, University Park, PA.

The early stages of heteroepitaxial growth of Co on Cu(001) are studied with \textit{ab initio} kinetic Monte Carlo (kMC) simulations, i.e. kMC with rates of the atomic processes calculated by density-functional theory (DFT). By employing the DFT-PW method for the PES calculations that show for low coverages Co adsatoms prefer to adsorb substitutionally as opposed to adsorption at a fourfold hollow site. Due to the exchange processes substrate adsatoms are generated on the surface. We find that the substitutionally adsorbed Co atoms act as nucleation centers both for on-surface Co and Cu adsatoms, the effect being stronger for Co. Further, we focus on the adatom diffusion of both species (Co and Cu) on the 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 to 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 homoeptaxial case (selfdiffusion of Cu on Cu(001)) and deviations from the predictions standard nucleation theory are discussed. The atomic exchange dynamics gives rise to dramatic changes in surface morphology and island density. The DFT-KMC results provide explanation of the \textit{bimodal} growth mode, recently observed in STM-experiments (Nouverté, \textit{et al.}, Phys. Rev. B \textbf{60}, 14882 (1999)) and characterized by a high density of small Co-islands and large, Co-decorated Cu islands.

10:30 AM P4.6
PROBING THE FPINS PHASE DIAGRAM OF FCC Fe ULTRATHIN FILMS USING CO ATOMS. John Pierce, Martin Terjôs, 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 (MORE) 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 in a function of temperature. We demonstrate this method on the face-centered tetragonal (fct) Fe/Cu(100) system, which undergoes a structural transformation to a face-centered cubic (fcc) phase at a thickness of 4 ML. Under ultrahigh 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 reverse magnetization from the direction perpendicular to the film to the in-plane direction. We find that the film thickness at which the spin would revert 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 these films, which maps the magnetic state (magnetization perpendicular, or in-plane) in the space of temperature and Fe thickness.

10:45 AM P4.7

We have developed a novel thin film processing method based on pulsed laser deposition to process nanocrystalline magnetic materials with an average 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 loops and low temperature magnetic properties 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 MRAGES. C. P. Lutz, D. M. Eigler, IBM Research Division, Almaden Research Center, San Jose, CA.

While the correlated electronics underlying the diverse manifestations of magnetism and spin have long been studied via microscopic 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 in atomic length scales, but to manipulate spins as well. This talk will detail new results that exploit these techniques using low-temperature scanning tunneling microscopy. We have directly imaged the electronic wave function and spin-compensation cloud formed around isolated magnetic moments on a metal surface. Utilizing the detection of this many-body state as 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 nanostucture. The "quantum mirage" thus cast by a single magnetic atom can be coherently reafered at a distinct point where it is detected as a proton atom around which the electronic structure mimics that of 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.

11:30 AM P4.9
ULTRAFAST MAGNETIZATION REVERSAL DYNAMICS ON A MICROSCALE 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 Ni$_{81}$Fe$_{19}$ microstructure (10µm x 2µm) is studied using time-resolved terahertz spectroscopy and low temperature magnetic 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 dominated 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 $f=1$ GHz is caused by damped precession of the magnetization vector, whereas another mode at $f=0.5$ 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 TPS.1
KINETIC EFFECTS IN EPITAXIAL GROWTH. J. Terrell, IBM T. J. Watson Research Center, Yorktown Heights, NY.

Epitaxial growth is controlled by an interplay between thermodynamic and kinetic driving forces. A change in 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 role 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 Rusch 3,4, Russel Cahill 5, Mark Gyure 6 and Andrew Zangwill 7. 1 Georgia Tech, School of Physics, Atlanta, GA; 2 UCLA, Dept. of Mathematics, Los Angeles, CA; 3, HRL, Malibu, CA.

The level set approach applied to the modeling of epitaxial growth allows a description which is discrete (atomic) in the height profile and continuous in the lateral dimension. Therefore, virtue of a 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 at a velocity that is determined 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.


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 depleted 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 the 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 EHLICH-SCHWOEBEL EFFECT FOR VACANCIES: LOW-INDEX FACES OF SILVER. Michael L. Hafel, Naval Research Laboratory, Washington, DC.

We employ surface-embedded atom-method potential to investigate the diffusion barriers of vacancies diffusing over and near steps on the low index faces of silver for vacancy formation, exchange via 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 (313 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 effects on vacancy island shapes and 3D pitting are discussed and contrasted with the usual ES effects on adatom islands.

2:45 PM P5.5
EPIAXIAL GROWTH OF SURFACE SELF-DIFFUSION ON GOLD (001) SURFACE. Mokio Doyama, T. Ohhme, Y. Kogure, Tokyo 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 and embedded atom method simulations. For example, the activation energies of ad-atom clusters on (001) plane of gold are calculated. It was found that the activation energy of the movement of an ad-atom on (001) of gold is 0.62 eV. These energies are calculated in two directions: in direction of a di-adatom 1.00 eV, and 0.63 eV from the first to the second nearest neighbor. The conversion energies of ad-atom clusters have been calculated. These were more than half of one electron volt and much smaller than the separation energy 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. Logan, 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 phase transition 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 more strongly influenced by the presence of oxygen. Conventional STM has been used to form well isolated islands from a substrate covered with thin layers of oxygen. In situ STM and LEED studies show that oxygen on the Ag[100] surface causes the typical phase transition at 320 °C, and adsorption isotherms are found to be consistent with previous measurements of adsorption on Ag[100]. The molecule growth and movement of adatom clusters at various temperatures are observed. The impact of oxygen on the growth of Ag[100] films is considered in this work.


4:00 PM P5.7

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 show that the alloying process proceeds via an extraordinarily interesting mechanism. During room temperature physical vapor deposition of Sn on Cu[111], similar to what is often observed in other cases of metal-on-metal epitaxy, the Sn quickly coalesces into 2D films immediately after the formation of the Sn islands, however, a striking and unexpected reaction sets in. Islands comprised of some 100,000 atoms room 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 expelled 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 DE-AC04-94AL85000.

4:15 PM P5.8

Using scanning tunneling microscopy (STM) and first-principles density functional-theory calculations to study submonolayer films of Ag-Co surface alloys on Ru[001], 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 nano-scale 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. Iván Díaz, John C. Hamilton, Sandia National Labs, Livermore, CA.

It has been shown by recent experiments that bulk immiscible metals (e.g., Ag/Cu, Ag/Co, and Au/Ag) 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 Pseudo-Koiterovtsov 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.


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 above 300K the antiparallel growth mode shows an observed oscillatory dependence on the growth temperatures during Ag deposition. Measurements show that the first-layer Cu atoms were shifted and localized in defined areas in which the stacking changed from ABC to ABC (hcp-sites).

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

P6.4 INVESTIGATING THE EFFECT OF THE β-Cr₂N TO CUBIC Cr₃N₉ PHASE TRANSITION ON STRESS STATE IN CHROMUM NITRIDE THIN FILMS. B.A. Rainey, S.M. Yalovoe and J.C. Bilello, Center for Nonlinear Systems, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI.

Several series of chromium nitride thin films were deposited by reactive sputtering over a range of deposition conditions to explore this transition. A number of these films with phase compositions varying from β₃ [hexagonal structure] Cr₂N to cubic [NaCl structure] Cr₃N₉ (x ≥ 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 Cr₃N₉ on film stress state. The film stress within the phase of growth (in-plane) was calculated from lattice curvature measurements obtained with double crystal x-ray diffractometry. X-ray diffraction (XRD) 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 Cr₃N₉ transformation. However, a transition in stress state is not observed in conjunction with the phase transformation in films grown in the other deposition geometry used in this study. We conclude that the tensile compressive phase transformation promotes a decrease in tensile stress whereas other factors contribute to the production of compressive stress in these films.

P6.5 SYNTHESIS OF SILICON OXYNITRIDE FILMS PRODUCED BY RADIO-FREQUENCY PLASMA ASSISTED ELECTRON CYCLOTRON RESONANCE. Jason Brewer, Avi Raweh, 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 as 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, B) 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 nitrogen layer thickness was observed at a N₂O ratio of 1 and V, B = 50 V. The nitride to oxide ratio in the grown layer was found to be dependent on the competitive processes between the O²⁻ and N⁺ species. At V, B < 20 V, a predominantly oxide layer was formed due to the relatively high concentration of O²⁻, while at V, B > 20 V the formation of the film proceeds mainly by NO and N⁺ ions and radicals. The effects of N₂O ratio, gas pressure, and V, B on the composition and properties of the fabricated films are presented.

P6.6 GROWTH OF EPITAXIAL Al₂O₃ FILMS ON SILICON BY IONIZED BEAM DEPOSITION. Sang-Woo Whang, Yun-Ki Choi, Hong-Kyu Jang, Chung-Nam 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 substrates 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/[111] Si with [110] Al₂O₃/[110] Si and [111] Al₂O₃/[111] Si with [112] Al₂O₃/[112] Si. The stoichiometry of the films was found to be similar to that of sapphire from XPS measurements.

P6.7 AN XPS STUDY OF THE EARLY OXYNITRIDATION STAGES OF IDEALLY HYDROGEN-TERMINATED (100) SILICON IN N₂ AND O₂ ATMOSPHERES. G. Corcelloni, S. Lecce, O. Vinciguerra, STMicroelectronics, ITALY. G.G. Condorelli, I.L. Fragni, Dept of Chemistry, Univ of Catania, ITALY.

The kinetics of oxynitridation of single crystalline silicon in the monocycle 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 misleading potential and relaxation effects the charge transfer associated with the oxidation was also determined.

P6.8 NANO-SCALE HETEROEPIKTAL CONTROL OF MAGNETIC OXIDE THIN FILMS ON ULTRA-SMOOTH SAPHIRE SUBSTRATES. S. Takakura, T. 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 magnetization of magnetic oxide films for constructing low dimensional structure. Here we report the formation of nanowires and nanocasts of [(Mn,Zn)] ferrite, Fe₃O₄ as ferrite materials and NO as an antiferromagnetic materials. These films were deposited on ultrasmooth 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 strain with step height of 0.2nm and terrace width of 10nm to 15nm. It is expected for nanocrystal filaments of substrates to enhance the epitaxial growth of the films and also step growth when the temperature is high enough for precursors to migrate to the step edges leading to formation of the nanowires and nanocasts. In the case of the (Mn,Zn) ferrite, thick films were grown epitaxially in the spiral growth mode, but ultra-thin films became nanowires (6.5nm high, 20nm wide) along the atomic step edges. The height of 6.5nm for nanowires is lower than the height of (Mn,Zn) ferrite (111) plane. By controlling the step height and terrace width of ultra-smooth substrates, the novel heteroeptaxy could be attained towards construction of low-dimensional structure.

P6.10 ON THE NUCLEATION MECHANISM OF s-CrN ON AN s-BN BASELAYER. Jian Xu and Hans Oehlschlaeger, Center for Materials Research and Institute for Surface and Thin Film Analysis, University of Kaiserslautern, Kaiserslautern, GERMANY.

The growth of CrN layers by rf magnetron sputter deposition on Si (100) has been studied in dependence of the rf 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 30nm
occurs when film thicknesses around 100 nm had been reached. When interrupting the deposition process before, during and after the period of negligible grain growth, AFM images revealed 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. Scatter 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 a more ordered crystal structure. The shrinking depths are in good agreement with the findings in the previous literature. The film formation occurs when the squared strain energy of the initial hBN layer exceeds that of a cBN film of equal mass but reduced thickness.

P.6.7 GROWTH OF AlN AND TIN STRUCTURES BY PLASMA-ENHANCED PULSED LASER DEPOSITION, Edward Pointdexter, 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 (λ = 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 substrates were found to be polycrystalline or amorphous depending on substrate temperature. In situ RHEED indicated that single-crystal TiN films were obtained on both types of substrates, however, the temperature range of investigation (500 - 800°C). AlN films deposited on ~200 Å thick TiN buffer layer on silicon were found to be polycrystalline. In contrast, ~600 Å thick single-crystal TiN film was grown on a (001) silicon substrate by using a ~20 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/silicide are atomically smooth with only one or two monolayer roughness. The epitaxial relationship of the film to the substrate is [110]AlN/[110]TiN/Au/Si [001]."
<111> //Si<111> in film normal direction and γ-Al₂O₃ //110> //Si //110> in film plane direction.

P6.13 GROWTH OF EPITAXIAL NICKEL OXIDE ON NICKEL BY OXIDATION. Mani Gopal, Michael Cima, Department of MSE, Massachusetts Institute of Technology, Cambridge, MA.

The increase in volume during the oxidation of nickel to nickel oxide is over 65%. This volume change induces a strain in the oxide film, relieved by the 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 90%. 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.


Thin film morphology and microstructure are very important because they influence properties relevant to applications such as solar-selective absorber coatings, 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. The growth of thin films of cobalt oxide on a variety of substrates from different metallicorganic complexes, under various growth conditions. For example, it is found that Co₂O₃ films grown from Co(H) acetate at low temperatures ~350°C on glass, quartz, and 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 epitaxial films grow readily at substrate temperatures as low as 450°C, the growth of nearly perfect epitaxial films of Co₂O₃ occurs on SrTiO₃(100). Under very similar CVD conditions, growth on 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 precursors) 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 Co₂O₃ thin films were studied by XRDR, SEM, AES, and AFM. Optical properties measured by spectrophotometry and ellipsometry will also be reported.

P6.15 FORMATION OF ATOMICLY FLAT SURFACES ON STRONTIUM TITANATE AND SAPPHIRE. A.P. Li, C. Bednarchuk, Z. Dai, and B. Gohling, Center for Sensor Materials and Department of Physics & Astronomy, Michigan State University, MI.

The SrTiO₃ (100) and α-Al₂O₃ (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 SrTiO₃ (100) and α-Al₂O₃ (0001). Atomic force microscopy has been used to examine the surface structures. As-received SrTiO₃ crystals were carefully cleaned and etched in a buffered NH₄F:HF solution to remove damaged layers. Well-defined and ultra-smooth SrTiO₃ (100) with unit cell height steps of 0.04 nm was obtained by O₂ annealing at 900°C. As-received α-Al₂O₃ (0001) crystals were chemically cleaned and then etched in a solution of NH₄OH, H₂O₂ and H₂O. With this treatment, facet formation on the surface was observed after annealing in the range of 900-1200°C in air for short periods. The strongly 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. Eswaren Dharmarajan, Wen-Jie Qi, Renee Nieh, Linggu Kang, Katsumori Onishi and Jack C. Lee, The University of Texas at Austin, Austin, TX.

The need for alternative gate dielectrics to replace conventional SiO₂ is increasing to facilitate further CMOS scaling. Various high-k materials like Ta₂O₅, TiO₂, ZrO₂, HfO₂ have been studied as potential replacements. However, it is thermodynamically stable in contact with Si and therefore requires some barrier layer. One of the most promising materials for use as an alternative gate dielectric is Sr Zr silicate due to its thermodynamic stability on Si and its good interface quality with Si. In this study, ultra-thin Sr Zr silicate films (~60 nanometers) 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 ZrO₂ and to have Sr rich films for better interface quality. Films were Rapid Thermal Annealed in N₂ 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 nanometers with gate leakage significantly lower than SiO₂ of similar thickness and hysteresis < 20mV. The films also exhibit high 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. Jin Hac and Tiesuan Lin, 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 polyimine[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 films were monitored by UV-visible spectroscopy, 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. References: 1. W.B. Stockton, M.F. Rubner, Macromolecules 1997, 30, 2714. 2. L. Wang, Y. Fu, Z. Wang, Y. Fan, X. Zhang, Langmuir 1999, 15, 1360.

P6.18 MODELING THE STRUCTURAL DISJOINING PRESSURE OF THE NEMATIC LIQUID CRYSTAL THIN FILMS. Aleksandar D. Roy, 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 Lappin’s interfacial stress balance equation. Identification of the interfacial stress tensions 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 components result in a disjoining pressure that may be disjoining or cojoining. Phenomenological expressions for the two structural disjoining pressures are obtained using the classical equations of liquid crystal bulk and surface elasticity.
GROWTH FRONT ROUGHENING OF ROOM TEMPERATURE DEPOSITED OLIGOMER THIN FILMS. D. Vroomans.

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 improve the electrical properties and the performance 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 their growth morphology. In this work growth front scaling exponents are investigated for PPV-type oligomer thin films vapor-deposited onto silicon substrates at room temperature. For film thickness d \sim 15000 nm, commonly used in optoelectronic devices, height-difference correlation function measured by atomic force microscopy yields roughness exponents in the range H=0.45 \pm 0.04, and a rms roughness amplitude s which evolves with film thickness as a power law s \propto d^{\beta} \sim 0.05. The non-Gaussian height distribution d and the measured scaling exponents (H and \beta) suggest a growth front roughening mechanism close to the described by the Kardar-Parisi-Zhang (KPZ) growth model.

SELF-ASSEMBLY OF COLLOIDAL PARTICLES ONTO SURFACES OF EMULSION DROPLETS. M.F. Hsu, M. Nikolaidis, A.D. Dimanou, A.R. Branch, D.A. Weitz, Department of Physics, Harvard University, 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 concentration 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.

GROWTH MECHANISM AND MORPHOLOGY OF FILMS PRODUCED BY VAPOR DEPOSITION POLYMERIZATION. Y.-P. Zhao, J.B. Forcin, 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 different reactions: 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 processes: after the monomers have condensed on the substrate. For the VDP process, the reaction occurs only at the end of a polymer chain, and surface diffusion, intermolecular interaction, and chain retraction 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 work, we examine the roughness evolution in the growth of simple polymers, -(CH2)n-, using a computer. 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 0.01, and the lateral correlation length \xi grows as \xi \sim d^{1/2}, with 1/2 = 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.

MOLECULAR ORIENTATION IN THE PEPTIDE SELF-ASSEMBLED MONOLAYERS. Kazuhiro Fujita, Ryuichi Yokoyama, Tetsuo Tsuchi, Kyoto University, Dept. of Applied Sci., for Electronics and Materials, Kyushu, 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 long dipole moment along the helix axis are considered candidates to control the electric property at the interface. Two kinds of helical peptides, Peptide I and II were synthesized. The structure and the orientation of the peptide group at the terminal and Peptide II at the terminal. Each peptide can bind on a gold substrate at the disulfide moiety, resulting in 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 were 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 SAMs was determined to the molecular length along the helix axis. The ratio of I band and II band in IR-RAS revealed that the peptide and component SAMs have much higher 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).

POLYMERIZATION OF MULTILAYER FILMS USING A SPINNING PROCESS. Jinhan Cho, Kookcheon Chae, Seoul National University, School of Chemical Engineering, Seoul, Korea; Jong-Dal Hong, University of Incheon, Department of Chemistry, Incheon, 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 carboxylic poly(ethylene glycol) (PAH) and amionic poly(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 is only 15 seconds. The spin-coating process of the spin-coated 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 laminarization 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 homogenous and smooth, indicating a surface roughness below 0.5 nm, as evidenced from X-ray reflectivity and atomic force spectroscopy (AFM).

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 (GBD) 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 formulation allows for an inhomogeneous charge distribution on this surface. In particular we perform extensive simulations to study the effect of layered surfaces - e.g. lattices - 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 copolymer grafted surfaces. It is also relevant to the protein crystal growth. This work was carried out under the auspices of the

P6.27
NUCLEATION AND GROWTH OF COLOIDAL HARD SPHERE CRYSTALS
Eric Granger, Eric R. Weeks, Daniel 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 image 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 small liquid 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 as well as the surface energy and the morphology of the crystal lattice.

P6.28
SELF-ASSEMBLY OF RUTHENIUM PORPHYRINS INTO MONOLAYER AND MULTILAYER ARCHITECTURES VIA HETEROCYCLOGENIC CHEMISTRY: DESIGN, SYNTHESIS, AND APPLICATIONS
Joseph 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. Matsuoka, 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 macrocycles 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 silicon substrates. Following exposure of the pyridine-terminated surface to the porphyrin, UV-visible 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 pyridyl spacer in solution, allowing coordination of additional porphyrin units. More highly organized systems are now being explored which utilize tetrapyridylmetalloporphyrins capable of coordination into larger planar arrays for subsequent incorporation into extended multilayer architectures. The morphology of these thin films can be controlled using AFM or TEM 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 on n-doped sapphire substrates of crystal orientation [0001] and [1120] (C- and R-plane Al2O3, respectively) has been monitored in situ and ex situ atomic force microscopy (AFM), contact angle measurements, and transmission infrared spectroscopy (IR). When annealed at 130°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 indistinguishable to the adsorption site at different sites, monolayer growth is demonstrated. Furthermore, from our characterization techniques we 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

The layer-by-layer deposition of conformal thin films from a variety of organic/inorganic materials proceeds to be a powerful technique in constructing multi-component molecular architectures with precisely controlled thicknesses. Our group has previously reported on the metallographic assembly of thin films using 88° dihydroxy 5,6-bisquinoline (bisquinoline) and diethyl zinc (as the zinc precursor). In this paper, we have utilized different zinc precursors (ZnEt2, ZnCl2, ZnBr2, Zn(CH3COO)2, and Zn(C2H5COO)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 size 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. Investigating the order within these assemblies was shown to decrease their photoluminescence efficiency.

P6.31
UNIQUE FEATURES OF THE CRYSTALLIZATION KINETICS OF FeCoBSi THIN FILMS OBTAINED BY LASER ABLATION DEPOSITION
M. Sorensen, A. Grabis, Duquesne University, Department of Physics, Pittsburgh, PA.

Pulsed laser deposition was used to obtain a metallic film in a thin film form using the amorphous Fe7Cr2B14Si2 ribbon as a target. Glass substrates were used. The as-deposited films were annealed under the same conditions as the ribbon samples in order to compare their crystallization behavior. Transmission Μo-, μ-X-ray measurements were performed to determine the crystallization products formed due to annealing of the Fe7Cr2B14Si2 ribbon. Conversion electron Μo-μ-X-ray 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 Μo-test spectra revealed the formation of both the bcc-FeSi and bcc-Fe3 (Si,B) phases in the bulk of the annealed ribbons. However, at the surfaces of the ribbons annealed at higher temperatures, the bcc-Fe, bcc-Fe3 (Si,B) and tetragonal Fe3B 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 500°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 iron-coring amorphous phase with hyperfine field of 518 T. The hyperfine parameters indicate that this phase could be Fe62O38. Our  Μo-X-ray study showed that the crystallization kinetics of the thin films of FeCoBSi is different from the crystallization mechanism of the bulk ribbon.

P6.32
LOW-FIELD MAGNETORESISTANCE PROPERTY OF La0.6Sr0.4MnO3 THIN FILMS WITH NANO-CRYSTALS EMBEDDED IN A JUGO MATRIX
Jianliang Liu, Jinjing Ling, Jinliang Liu, Nanjing University, Laboratory of Solid State Microstructures, Nanjing, CHINA.

La0.6Sr0.4MnO3 (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. Film crystallinity does not largely depend on the deposition temperature. Significantly enhanced low-field magnetoresistance for the films 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 LATHANUM STRONTIUM COBALTITE ONE THIN FILMS FROM A PHOSPHUS MELT
Hayuee Chong, Yi Dong, Lawrence Berkeley National Laboratory, Berkeley, CA; Sangye Chen, Chonglin Chen, Paul CW Chu, Dept of Physics, University of Houston, Houston, TX.

It is well-known that La2/3Sr2/3CoO3 (LSCO) is a good conductor. 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 between room temperature and the glass transition temperature, the amorphous thin films become metallic and look 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 a glassy to a crystalline state. X-ray diffraction studies show that the annealed films are on [001] LaAlO₃ (LSCO) and they tend to grow in a cube-on-cube fashion on LSO.

P6.34

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

Orthorhombic β-FeSi₂ behaves as semiconductor with a direct band gap of about 0.95 eV, and shows a large photoelectric 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 cell. 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 Si were used as substrates. The substrate temperature was 500°C, and the laser power was 20 W. The result of XRD measurement showed that the film grown on Si[111] substrate was in a polycrystalline state, while thin films grown on Si[110] substrate were monocrystalline. The band gap energy calculated from the results of transmittance measurement was about 0.75 eV. This value is smaller than that 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 AI FILMS.** C.A. Volkert, and S. Bühler, Max-Planck-Institut für Metallforschung, Stuttgart, GERMANY.

The effect of surface topology 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 prismatic 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 the grains in the uncompressed region. 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 SUPERIORIC PbSnF₄.** INFLUENCE OF THE REACTION MEDIUM AND PHASE TRANSITIONS, AND RESULTING ANISOTROPIC PROPERTIES. Georges Défago and M. Céline Médard, Concordia University, Dept. of Chemistry, Laboratory of Solid State Chemistry and Microwave Spectroscopy, and Laboratories for Inorganic Materials, Montreal, 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 improve the PbSnF₄, by choosing the right medium and phase transitions, and resulting anisotropic properties, or with full disorder, resulting in cubic unit-cells and no superstructure. In ordered phases, the tetrahedra of lead ions and fluoride are not perfectly ordered, and its evolution through the α- to α'-PbSnF₄ phase transition, where the minterm of the transition reduces the alignment. The implications on the mobility 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 \(\text{Si}_3\text{N}_4\) formation in conventional thermal silicon dioxide \(\text{SiO}_2\) films by dual-frequency plasma were studied. The nitridation of the \text{SiO}_2 films was performed in nitrogen plasma sustained by radio frequency and microwave discharge and for electron cyclotron resonance. The effect of the nitridation time, substrate temperature, and gas pressure on the nitrogen content and on the \text{Si}_3\text{N}_4 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 \text{Si}_3\text{N}_4 cycled around 30 min of nitridation. This time was found to decrease while 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 the high nitrogen concentration gradient on the nitrided surface. FTIR analysis indicated that the nitrided films were composed of \text{Si}_3\text{N}_4, \text{SiO}_2, and \text{SiO}. AES analysis revealed that the N/(Si ON) ratio in the nitrided layer was higher for films nitried by ECR/RF plasma when compared with those nitried 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 NiTiH THIN FILMS.** Chen Zhang, Ralph H. Zee, Auburn University, Materials Research and Engineering Center, Auburn, AL, Paul E. Thomas, Johnson Controls, Inc., Corporate Technology, Milwaukee, WI.

The microstructure evolution of Ti-rich NiTi thin films and (Ti,H)-rich NiTiH thin films containing 9% H was investigated. These films were deposited from single NiTi and NiTiH targets using a DC magnetron sputter system. Two single-crystal silicon substrates were obtained by using single crystal silicon substrates. The thickness of these films was controlled between 10-12 μm. In this investigation, the effects of deposition temperature on the surface and cross-sectional microstructures of these films were studied. Surface 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 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 determined using x-ray diffraction. All the 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 μm to 2.5 μm, 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-HELL TIGHT-BINDING MOLECULAR DYNAMICS**
SIMULATION STUDY ON THE CHEMICAL VAPOR DEPOSITION
PROCESSES. Seichi Takami, Hiroshi Kurokawa, Ken Suzuki, Muneji
Akita, Akira Imamura, Hiroshi Kokumai, Gaku Matsumi, Depmt.
Of Materials Chemistry, Sendai, JAPAN; Akira Imamura, Hiroshi
Kokumai, Gaku Matsumi, Sendai, 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
methods including chemical vapor deposition processes. The
management 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 electronic state
with a considerable reduced computational load. In addition, this
program can handle both set-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 SiI radicals on a Si(100) surface.

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

The model suitable for simulation of CVD growth of amorphous Si
and SiOx is proposed. It is based on the network properties of the
materials and essentially involves dangling bonds arising during the
real process. Interatomic interaction is described within Kesting-like force
model (P. N. Kesting, Phys. Rev. 145, 637 (1966)) with additional repulsive
force between nonbond 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. NDF calculated for the simulated amorphous silicon and silicon 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 SiOx). Porosity in amorphous Si is
quite low (< 2%) almost regardless the nitrogen sites density (NSD)
on the substrate surface and is associated with structural defects
(local breaking of chemical bonds). Silicon 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. Yanbing Sun, Song-Yong Lee,
Nicholas Nguyen, John G. Ekerdt, John M. White, The University of
Texas, Texas Materials Institute, Austin, TX; Ismail Emeish,
Motorola, Advanced Products Research and Development Laboratory,
Austin, TX.

Low temperature chemical vapor deposition of tungsten films on
SiO2/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
W(CO)6 precursor over temperatures ranging from 250 to 500°C.
These films contain approximately 10% C and 6% oxygen as
determined by XPS. The growth temperatures were consistent with
pyrolysis studies that indicated W(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 a polycrystalline microstructure, and the grain size increases
dramatically as the growth temperature increases. The carbon and
oxygen chemical states indicate carbidc 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 graphic
cap and carbonization films 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 GÀNEPLIERS GROWTH MECHANISMS

USING IN-SITU REFLECTANCE IN MOCVD. O. Brizz, M. Moret,
S. Raffournier-Gir, L.L. Aumolard 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 is now to the excellent degree following the 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 better reproduce high quality 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 buffer-growth and growth). Additional reflectance
measurements (AFM and MEB) were performed at different stages of the
growth process to ensure additional information. As a result, we demonstrate that the characteristic 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 ATOMIC SIMULATION STUDIES OF PLASMA-ENHANCED
CHEMICAL VAPOR DEPOSITION OF HYDROGENATED
AMORPHOUS SILICON FILMS. Shayan Ramalingam,
Bhimanagiri Srinivas, Fang Y. Aydil, and Dimitrios Manos,
Department 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 [SiH] surfaces from silane containing plasma. Special emphasis is placed on the identification of the
elementary surface chemical reactions that govern the deposition
process, the amorphous growth mechanism, as well as the structural and compositional charaterization 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
calculated along the reaction path based on molecular-statistics
calculations and the energy levels of reactants, transition-state, and product configurations are computed accurately based on
density-functional theory. Our MD simulations reveal a broad class of
transition reactions which play important roles in the amorphous film
deposition process. Silicon incorporation into the growing film occurs through transition reactions into Si-Si bonds with H radicals.
Surface hydrogen can be removed by abstraction according to Eley-Rideal mechanisms or through a Langmuir-Hinshelwood mechanism that involves formation and dissociation 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 trilithides and surface disilane species. The surface structure, surface chemistry, and hydrogen
content, roughness, surface reactivity, and surface composition analysis was 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
hydrogen content also 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 EPI-TEXT.
AND OVERGROWTH OF AN INTEGRATED LASER/
MODULATOR QUANTUM WELL STRUCTURE USING MOVPE AND
MOVPE. Philipp Kröner, 1, 2 H. Bräuninger, 1 R. Gesnner, 1
J. Riegler, 1 M. Schier, 1 E. Veuhoff, 1 O. Marti, 1 H. Heinrich.
Institute of Applied Technology, Corporate Research CEPH, Munich,
GERMANY; University of Ulm, Dept. of Experimental Physics, Ulm,
GERMANY.

Laterally integrated laser/modulator structures for 1.55 µm wavelength form a desirable platform for high bandwidth optical
data transmission. A three-step epitaxial process involving the separate growth of the laser and the modulator structure, finally
overgrown with a common clad, allows for independent process
optimization. Here the MOVPE growth of the quantum well (QW)
linewidth structure on a (001) InP substrate is
applied, a SiNx stripe mask is deposited and 400 nm deep trenches are etched into the mask openings by reactive ion etching. Following a wet chemical etch to remove the remaining glass, the SiNx mask is removed. The electron-beam deposition modulator structure is selectively filled into the trenches by MOVPE. As a major focus we will present the role of the trench wall profile, surface restructuring induced by surface mass transport phenomena, microcrystalline and polycrystalline growth, and the influence of growth rates and V/III ratios for quantum wells and all other layers. Optimizing those parameters allows for a phonon bath coupling to the InAs layer. Growth nonuniformities can be limited to a stripe of 500 mum width. The main factors to be minimized from the InAs deposition onto the trench were the following: the thickness losses from the trench and 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, an etching inducing 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. Makhopadhyay, and S. Sivashankar, 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 clarify these aspects of MoCVD processes by growing films 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 aluminium β-diketonate complexes were used as the CVD precursor. We have studied nucleation, and growth rate 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 TEM. The chemical composition of the films and of the film surface interface was determined by Auger depth profiling. Carbon present in the film directly affects the optical properties of thin films, which has been 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 has been carried out on the lattice-gas model wherein atoms having unit volume occupy a unit cell of the substrate. A reaction rule on the substrate was taken 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 SI:ON FILMS.戴辉 (Beau) Khanna, R.J. Gambone, State University of New York at Stony Brook, Dep. of Materials Science, Stony Brook, NY; N. Goldobin, Standard MSMS 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 required, requiring a lower temperature zone from 550-600°C. In this study polysilicon films were grown in a hot-walled LPCVD reactor at 500°C to a thickness of 450 nm on p-type silicon substrates. The tensile as-deposited stress in the films was then measured with a deflection of 500 Hz, the stress 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 (~1x10/cm²) 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 underlying behavior is discussed.

P6.49
MODELING MoCVD: THE GROWTH OF MoCVD THIN FILMS. Takao Shima, Leberth V. Khan, Courant Institute of Mathematical Sciences, New York University, New York, NY.

YBaCuO thin film growth by metal-organic 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 Scholle and E recently. Here we carry out a numerical study of a phenomenological model with optical and kinetic terms, to that of Scholle 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 means 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 in the model at the same time. Films that are initially rough are observed to coarsen with time.

P6.50
XRAY SCATTERING STUDY OF CHEMICAL VAPOR DEPOSITION GROWTH OF SiC THIN FILMS: R. Ramesh, G. B. Steinhoff, J. S. Brandon, J. A. Eastman, A. Oudjello, G. R. Bii, 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, Argonne, IL.

Thin films of Pb (Zr1-xTi2x)O3 and related perovskite materials have attracted much attention for integration into a variety of microelectronic applications, including nonvolatile memories, pyroelectric imaging devices, and microelectronics/sensors/actuors/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 sensitive probes. As a model system, we have investigated PbTiO3 homeopitaxy and heteroepitaxy on SrTiO3(100) substrates using in situ 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 layered-layer fashion on SrTiO3 at 650-750°C. The films grow coherently (in-plane lattice parameters matched to the substrate), resulting in a tetragonal distortion of the unit cell. Homeopitaxy 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 electron microscopy studies. This work was supported by the U.S. Department of Energy, Office of Science, under Contract W-31-109-Eng38, and by the State of Illinois under HECA.

P6.51
INVESTIGATION OF THE LAYERED STRUCTURE OF POLYCRYSTALLINE DIAMOND THIN FILMS GROWN BY ECAL-ASSISTED CVD BY SPECTROSCOPIC PHASE MODULATED ELLIPSOMETRY. Samuel G. Winter 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 (SMPE) from the near IR to UV range (830 nm-270 nm). By applying the conventional Bruggeman effective medium approximation (EMA) model and linear regression in the ellipsometry data, we obtained details about the film microstructure: [i] the microlayer structure and the effective thickness of the films; [ii] the volume fraction of the components (sp3 C, sp2 C) and of voids [3]; [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 modeling were compared with those obtained from other techniques. Micro-Raman spectroscopy was used to examine the relative amount of the different carbon content in the films and their polycrystalline quality. Atomic force microscopy (AFM) measurements validated the estimated roughness found at around tens of microns. This research work is supported from the Department of Energy (DE-EG03-99ER54579) and the University of Puerto Rico (UPR FIPI Grant No. 880344).

P6.52
EFFECT OF SULFUR ON CVD GROWTH OF DIAMOND (100). Hirohiko Tomura, Yui Zhou, Seichi Takami, Momoko Kubo and Akira
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. Aims to semiconductor, 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 boron, nitrogen, and phosphorus, therefore, its development is crucial to realize the diamond devices. Recently, an n-type diamond has been obtained by chemical-vapor deposition (CVD) using [H1101]2H2 mixture [1], where sulfur is thought to 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 C-C bond on the top of the 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. Tan, H. Hamada, T. Suzuki, and T. Ando, Phys. Rev. B, 60, 2139 (1999).

P6.55
CHARACTERISTICS OF LASER-ABLATED PLASMA AND PROPERTIES OF DIAMOND-LIKE CARBON FILM IN PULSED LASER DEPOSITION. Shuichiro Morimoto, Tomoki Ijigami, Kenji Ebinuma, Kumnomo 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 tools to diagnose the ablation process [1] are powerful tools to understand the DLC plasma, and are useful to establish correlation between plasma composition and properties of deposited films. In this paper, we describe systematic studies using OES [2] and LIF on the plasma plume 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, Csp², and Csp³ 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 C/C2 emission intensity ratio, which is greatly dependent on the target crystallinity and the laser energy density. It is suggested that the C2 molecule in the ablated plasma may not play an important role in producing high quality DLC films.

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

Cross-sectional high-resolution transmission electron microscopy (XHREM) 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 Ir interlayer was used to improve the adhesion of the Ni substrate. Diamond was grown using seeding and multiple process [1]. The Ir interlayer was used as a substrate. The 100Å Ir interlayer was used to overcome the deamination of Ni from the MgO substrate. Diamond grew without peeling and nucleation problem. The nanohardness of the bulk modulus of crystalline diamond, the results of computations are in agreement with experimental measurements.
combination of these techniques allowed to illustrate the diffusion paths and preferences in diffusion of various coating and substrate elements in both the temperature dependent and independent experiments. The coating comprises a 2µm thick TiAlCrYN coating on top of a 0.25µm thick TiAlCrYN base layer. In the as-deposited sample yttrium was uniformly distributed throughout the coating. The coating was heat treated at 700°C for 8 hours in vacuum to grow yttrium containing mixed elements and chromium mainly at column boundaries in the base layer. In contrast no evidence of substrate elements could be observed in the TiAlCrYN coating suggesting 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 0.25µm 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

Wednesday Morning, November 29, 2000
Room 203 (Hyne)

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 experiments of Quartz Crystal Microbalance (QCM) in recent years has 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 adsorbed molecules. We have thus combined a STM and QCM to allow direct imaging of films adsorbed on the QCM electrode under both static and oscillating conditions.[2] The results of these studies will be described, along with a discussion of whether our current knowledge of the fundamental properties inherent to the adsorbate/surface interaction is sufficient to enable more detailed control of adsorbates on surfaces through frictional drag forces.

Supported by NSF and ARO (DAEDALUS).


9:00 AM P7.2

SURFACE SMOOTHING CONTROLLED BY DIRECT EXCHANGE WITH BULK VACANCIES IN NAI1 K.F. McCarr, J.A. Nobel, N.C. Bartelt, Sandia National Laboratories, Livermore, CA

We have examined the kinetics of island decay on the NAI1(110) surface using low-energy electron microscopy (LEEM). Remarkably, the decay rate is constant in time and totally independent of the local environment (e.g., the width of the island, density of step 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 increased. For a temperature increase, the surface steps advance. For a temperature decrease, the surface steps retreat. The surface steps advance (retreat) in bulk vacancy concentration for a temperature increase (decrease). Remarkably, the size change accompanying a temperature change is strongly 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 derives 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 Science.

9:15 AM P7.3


In certain cases, the incidence energy of constituent atoms activates an atomic insertion mechanism, which decreases the surface roughness of metal thin films. In an effort to probe this effect, hexagonal copper films were grown in ultrahigh vacuum using an 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 grown until the beneficial effects are obscured by adsorb/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)/2x1 SURFACE. Ayako Ishimura, Miwako Suzuki and Shunmoku Nakada, Nanyo University, Dept of Quantum Engineering, Nanyo, JAPAN

Silicon mounds formed on the Si(100)/2x1 surface have been observed by STM at substrate temperatures of 500°C. The mounds have been fabricated by using STM tips. The shape of the mound pyramids 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 D₅ step. Just after the fabrication, the pyramids begins to decay immediately layer-by-layer. During the decay, the area of the bottom single layer of the pyramid is grown toward the dimer row direction which is perpendicular to the D₅ step. The layer width does not change toward perpendicular to the dimer rows parallel to the S₄ step. The area of the topmost layer of the pyramid decreases toward perpendicular to the dimer rows, because the both S₄ step edges are pinned by the step edges of the lower ones. Therefore the D₅ step and S₄ step edges 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 S₄ steps are fluctuate very much and knobs of the S₄ step edges are also moving. The ratio of the mound oscillates between about 2.5 and 1.5. The mounds detached atomically at the S₄ step edges and reached the S₄ 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


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 migration of 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 [1] 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. This channel we focus on in the GaN(0001) surface. For GaN it is the very Ga-rich conditions optimal for growth, a metallic layer-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. This metallic adlayer structures strongly affects the adatom sites, the migration paths, and the diffusion barriers. For the In adlayer structure we show that the adatom adsorption site for N adatoms is inside the metallic double layer and that adatoms diffuse between

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these two layers. The calculated diffusion barrier for subsurface diffusion is 0.5 eV, compared to 1.3 eV for surface diffusion [2].


10:15 AM \#P7.6

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 formation of the cone, the total 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 at high temperature 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 crystallite and the chemical potential change induced by the temperature jump provides a quantitative description of the structural evolution. The mechanism of ferroelectric 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 rotation. \*Work supported by the UMD-NSF MRSEC.

10:45 AM \#P7.7
ROUNDETAGE DUE TO EDGE DIFFUSION FOR IRREVERSIBLE AGGREGATION. \textbf{C. H. Houchens,} \textbf{M. Kang,} \textbf{M.C. Wheeler} and \textbf{R.E. Caflisch}, \textbf{UCLA,} \textbf{Los Angeles, CA; M.P. Gurel,} \textbf{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 melt phase are defined by the level set function \( \phi = n \), where \( \phi \) 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 the edge diffusion enhances surface roughness of the island boundaries in competition with the depolarizing field governs the kinetic 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 rotation. \*Work supported by the UMD-NSF MRSEC.

11:00 AM \#P7.8
STEP WANDERING ON SURFACES WITH MULTIPLE STRUCTURAL PHASES DURING GROWTH. \textbf{Hiroki Hirose,} \textbf{Toshikazu Ogin,} \textbf{NTT Basic Research Labs, Kanagawa, JAPAN; Changyou Hu, Ignatius S.T. Tsong,} \textbf{Arizona State Univ,} \textbf{Dept of Physics and Astronomy, Tempe, AZ; Mikio Uwaha,} \textbf{Nagoya Univ,} \textbf{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 two sides of the step. The degree of 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 \textit{ex situ} AFM and \textit{in situ} UHV-SEM. The step configuration after growth dramatically changed around the phase transition temperature between 1x1 and 7x7 after 20nm-thick Si layers were grown. Steps remained fairly straight on the surface covered with only 1x1 or 7x7. However, on the surface where both 1x1 and 7x7 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 1x1 and 7x7, the steps preferred to prostrate at the position in contact with 1x1. This suggests that more atoms diffuse to the step through 1x1 than through 7x7. During the phase transition, the tendency on the upper and lower sides of the area covered with 1x1 and 7x7 are different. Therefore, the difference in the mass transport on 1x1 and 7x7 causes the asymmetric atom incorporation. These step wandering phenomena during growth transitions often occur at steps, and adatom-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? \textbf{Jason T. Eastman,} \textbf{Y-P. Zhao,} \textbf{T.-M. Liu,} \textbf{G.-C. Weng,} \textbf{Resena Heller,} \textbf{Polytechnic Inst, Dept of Physics, Applied Physics, and Astronomy, Troy, NY.}

The Konigus-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 growth rate is 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, because the growth rate is very uniform. Conformal growth 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 shallow 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 elastic 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 strong density condition, which usually is not experimentally feasible.

Work supported, in part, by NSF.

11:30 AM \#P7.10
HETEROEPIAXIAL GROWTH MODE TRANSITIONS IN THE PRESENCE OF A SCHWOEBEL BARRIER AT AN ISLAND EDGE. \textbf{Vladimir I. Trofimov, Vladimir G. Mirokov,} \textbf{Instit of Radiophys & Elec STITAS,} \textbf{Inst 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 kinds of 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 real densities of adatoms and 3D 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 coarseness 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 in core) is strongly depending 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 small deviation of smooth growth in the first layer (LEEM) and SML after deposition about 5-10 monolayers it requires an universal scaling form and corresponding exponents are determined. [1] I. V. Trofimov, V. G. Mirokov, Comput. Materials Science 17 (2000) 510
SESSION P8: QUANTUM DOTS AND QUANTUM SIZE EFFECTS
Chun Ji N. M. Shen
Wednesday Afternoon, November 29, 2000
Room 302 (Hynes)

1:30 P M 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. Keaven, Department of Physics, Univ. of Oregon; H. W. Yoon, Dept. of Physics, Yonsei Univ.; I. Misuza, T. Ohkta, Dept. of Chemistry, Univ. of Tokyo; T. Shibata, 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: 3x1 Br/Si(111) [1] and 4x1 In/Si(111) [2], two metal adorbate 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 electronic band structure, the In/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 4x2 symmetry at low temperature. [1] J. Schaefer, E. Rotenberg, and S. D. Keaven, submitted to Phys. Rev. B. [2] E. Rotenberg, I. Misuza, K. Horikoshi, J. Schaefer, C. M. Lee, S. D. Keaven, T. Ohkta, T. Nagao, and S. Hasegawa, Phys. Rev. Lett. 82 (24), 4888 (1999).

2:00 P M P8.2
DISPERSSION OF QUANTUM-WELL STATES IN ULTRATHIN Al FILMS ON Si(111). Lucin Aballe, Celia Rorgero, Shaibin Gohale, and Karsten Horn. Forschungszentrum Jülich, Jülich, GERMANY. 2Physic 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 dependence of the electronic structure of aluminium films on Si(111). X7 using angle resolved photoemission, we observe the Al/Si interface is of intermediate thickness and homogenous interface and leads to the growth of two-dimensional Al[111] overlayers of good crystalline quality. We assign this to reduced diffusion and more homogenous nucleation during the early stages of film growth. Experiment and substrate temperature and above, the films are highly stable and improve their crystalline order while retaining their 2D character, and the interface remains homogenous, in contrast to the films grown directly at room temperature. The high quality of films deposited at low substrate temperature permits the observation of overlayers 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 line shapes. 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 overlayers 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 P M P8.3
CAPPING AND ORDERING OF InAs QUANTUM DOTS ON GaAs(001). J. Falta, Th. Schmidt, Institute for Solid State Physics, Bremen, GERMANY; K. Zheng, Ch. Heyn and W. H. Hams, Institute for Applied Physics, Hamburg, GERMANY.

We have performed measurements of grain incidence x-ray small angle scattering (GISAXS) and grain incidence x-ray diffraction (GIXRD) on InAs quantum dot arrays 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. Evaluating GISAXS for these samples, we find a preferential ordering of the quantum dots array in [110] and less pronounced in [110] 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 cappd 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 ordering conditions. The flow to determine the stacking of the dots. Under growth conditions, we find the dots to consist of an octagonal base with |111| and |100| side facets. GIXRD shows a partial relocation 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 P M P8.4
ORGANIZATION OF SELF-ASSEMBLED QUANTUM DOTS IN SiGe/Si MULITLAYER STRUCTURES: EFFECTS OF STRAIN AND SUBSTRATE CURVATURE. P. Sutter, E. Muirwa, 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 growing large-scale arrays of quantum dots. The proposed usage of such epitaxial quantum dot arrays 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 of 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 organization. Nonuniform strain on the planar surface was identified as the driving force for the observed improved ordering in such multilayer structures. 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. P. Sutter, J.C. Bean, and M.G. Lagally, Appl. Phys. Lett. 71, 3233[1997]. J. J. Tersoff, C. Teichert, and M.G. Lagally, Phys. Rev. Lett. 76, 1675 (1996).

2:45 P M P8.5
QUANTUM WELL PHOTOEMISSION SPECTROSCOPY OF ATOMICLY UNIFORM FILMS. J.J. Poggianti, Physics Department, University of Notre Dame, INDIANA; T. Miller, D.-A. Lii, and T.C. Chang, 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 photo hole by traditional methods is often unclear. In this work, we show that the photoemission technique is involved in the photoemission process itself. The observed peak width of the direct transition peak does not contain information on the lifetime of the photo hole, including electron-photon coupling, but also contributions from the band dispension of the initial state, simple inhomogeinities, 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 uniform films, as widely demonstrated in the literature. Electron states confined in thin films also qualitatively as two-dimensional electronic 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 sequence we are able to produce thin films of Ag identified enough for this technique on uniform films are possible. The high quality films allow the
observation of quantum well features in the s-band and the d-band of Ag as function of film thickness. The signal from individual atomic layers in detected by the fractions of monohary signatures in the spectra. The observed spectral features are analyzed with respect to the line shape and peak position as function of temperature,4 and photon energy employed in the experiments. Leading to detailed information on the electronic band structure of Ag.

3:30 PM *PS.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 nanoscale formed at QPC tunnel through the Fermi sea 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 EBM TO project at Japan Science and Technology.

4:00 PM *PS.7 DISPERSION AND QUANTUM CONFINEMENT OF ANISOTROPIC Ag(110) SURFACE STATES AT STEPS. J.J. Pascual, Z. Song, J.J. Jackiw, H. Conrad, K. Horn, H.-P. Rust, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, GERMANY.

Here we present the first dispersion measurements with scanning Tunnelling Spectroscopy of surface states (SS) centered at a Brillouin zone boundary: the 1 point in Ag(110). With a 4K-STM we analyse the oscillations in the charge density as the wave function scatters 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 [1]. The states at this energy have a one-dimensional character, and they propagate for long distances. Our evaluation of the E(k||) dependence shows that the bands exhibit an approximately parabolic dispersion, affected at high energies by the continuum of bulk bands near the 1 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 disperse 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 *PS.8 DIRECT PHOTOEMISSION FROM IMAGE POTENTIAL STATES OF Ag(111) FILMS GROWN ON W(110) BY VAN DER WaALS EPITAXY. Christian Pottenkamer, Hahn-Meitner-Institut, Berlin, GERMANY, Andreas Otto, IPkM, Heinrich-Heine-Universit鋞 D黚elme, GERMANY.

Layered compounds of the transition metal dichalcogenides facilitate the epitaxial growth of heterocontacts despite a large lattice mismatch. Films grow amically ordered with their own lattice constant on the hexagonal (001) substrate. The electronic properties of the junction turned out to be ideal, they seem to follow despite a small correction due to interfacial dipole the electron affinity rule, which is explained by the nonreactive and inert surface of the layered compounds. The forming of stacking defects at the contact plane. Ag grows on the (001) so called van der waals plane of W(110) amically ordered islands exceeding a clean (111) surface to vacuum. Accordingly a LEED pattern showing the 3-fold symmetry of Ag(111) is observed in photoemission with 21 eV in normal emission. At the Schottky barrier the secondary electron photo voltage is generated by the 21eV photons recognized by a shift of the Ag emissions with respect to the substrate. By excitation with photon energies in the range of 3.85 eV a strong electron emission below the threshold (determined by the macroscopic work function of Ag(111) and the substrate) is observed which is attributed to a resonant excitation of electrons from to image states n=1 and n=2 of the Ag (111) as a final state. An emission due to SPPE is ruled out. Tentatively we explain the subthreshold emission due to the formation of a triple junction at the Schottky barrier Ag/W(110) 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 *PS.9 CRITICAL THICKNESSES AND QUASIPERIODIC SUPER-STRUCTURES OF ULTRATHIN Ag OVERLAYERS ON [110] SURFACES OF III-V SEMICONDUCTORS. Ph. Ehret, Institut fiir Festkoerperforschung, Forschungszentrum Julich, Julich, GERMANY and Dept. of Physics, University of Texas, Austin, TX; C.K. Shih, Deps. of Physics, University of Texas, Austin, TX.

Ultrathin and atomically flat metal overlayers can be grown on many semiconductor substrates using a two-step procedure, but 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 155 K followed by annealing at room temperature. Scanning tunneling microscopy images and low-energy electron diffraction pattern show that Ag films obtained on GaAs(110) are all well ordered, atomically flat, and exhibit specific critical thicknesses, which are a function of the substrate material. In contrast, Ag films on InAs(110) substrates are increasingly disordered, although they are very flat compared to films grown at elevated temperatures. The [111] oriented Ag films on III-V semiconductors and III-Vphosphides exhibit two-fold superstructures, whereas on III-arsenides 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 is ascribed to a model 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, phonon defects, and domain walls. The effect of different substrates on the critical thickness, 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, P. Ku, 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 NANOASSEMBLIED 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 clusters catalyze oxygen reduction reactions with Au, to have a smallest active size. In contrast to the high selectivity of Pd(111) surfaces for the cyclodimerization of acetylene, small supported Pd 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 C2H4.

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, Donn Gibbs, Brookhaven National Laboratory, Upton, NY.

LaAlO3 is a perovskite oxide extensively used as a substrate for superconductor thin film growth. Previous observations had suggested a reversible change in the surface stoichiometry of LaAlO3 between room temperature and 250°C, but no detailed 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 different 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 concurrent (although smaller) movement of the aluminum atoms in the bulk. At higher temperatures, the atomic motions in the oxide thin films are accompanied by more radical structural change. In particular, the aluminum atoms in the thin film move more than one atomic diameter into the bulk (0.18 Å of a unit cell) changing from a five coordinated position to a pseudo-tetrahedral site. This is further supported by the fact that the simulated structure at the highest temperatures more closely resembles the experimental structure (185 K).

Highly ordered films of organic molecules on inorganic substrates are presently subject for investigations aiming to improved properties of organic electronic devices. Organic molecular beam epitaxy (OMBE) has proven to be one of the most attractive routes to achieve films of high structural quality. However, since molecule-substrate interaction may overwhelm molecular-molecule interaction by far this may lead to highly disordered, but strongly strained films with structures commensurate with the substrate surface. Polymeric thin-films (PCDA) 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 PCDA. Significant differential chemical shifts in UPS and NEXAFS reveal that the bonding is chemisorptive. However, films grown at low substrate temperature (< 150 K) show different electronic spectra, which transform into the RT spectra upon annealing. This indicates the adsorption of PCDA 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 (HREED). 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 (< 150 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, PCDA films can deliberately grown either in a strained epitaxial (i.e. substrate controlled) or in a bulk like structure due to the existence of a precursor.

9:30 AM  **P9.4**  
**GROWTH OF MULTICOMPONENT FILMS FROM ORGANIC METALLIC PRECURSORS. MONTE CARLO SIMULATIONS.**  
Chunyan Yu, University of Michigan, Dept. of Materials Science & Engineering; M. David Schuster, Princeton University, Materials Science & Engineering. Princeton, NJ.

Organometallic vapor phase epitaxy (OMVE) is a leading technique for the deposition of multicomponent ceramic films. At present, quantitative relationships between OMVE reactor conditions and film structure are poorly understood. In this presentation, we describe the development of a novel Monte Carlo simulation method for OMVE and apply it to the growth of two component A$_2$B$_3$O$_9$ 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 the 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 shown to grow in a manner similar to that observed for single crystal thin films. 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 microcrystalline phases (APBs). The observed 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 OMME growth of the ferroelectric oxide SrTiO$_3$. A two-body central force model potential is used to calculate binding energetics and surface diffusion rate constants. Implications of these results for understanding OMVE more generally are discussed.
LOW-DIMENSIONAL DEFECT STRUCTURES OF NaCl(100) FILMS. Christian Schlegelkamp, Winfried Ernst and Herbert Pführ, University of Hannover, Hannover, GERMANY.

We have investigated the morphological and the reactivity of epitaxially grown, monocrystalline NaCl(100) using LEED, UPS, EELS, and TDSD. The generation of NaCl steps proceeds 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 10%, was confirmed for the monocrystalline particles. The diffusion of NaCl steps with single atomic height, can be increased significantly by adsorption of 0.5 ML Si at 470 K.

In dependence 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 [100] orientation, the NaCl film grows below 200 K layer-by-layer forming polar steps along the [011] direction.

To characterize these structures, in comparison to defect-free NaCl(100) and NaCl films covered with F-centres, both the bond structure and the desorption behaviour of CO₂ has been investigated. The financial support by the Kuli & Salz Gmbh, Germany, and in addition by the University of Maryland/MBESEC, USA, is gratefully acknowledged.

CONTROLED NUCLEATION AND GROWTH OF NOBLE METALS ON POLYMERS. Vladimir Zaporozhenko, Knut Behnke, Axel Thrun, Thomas Strunkusk, and Frank Engel, Kiel Univ, 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 known as potential low-permittivity (low-k) dielectrics for on-chip interconnections. Therefore much effort has been made to understand and control the interfacial microstructure. The structure and properties of metal-polymer interfaces depend 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 density and growth morphology 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 205 (Hynes)

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

The electronic properties of thin metallic films strongly depend on their 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 of Pb recrystallisation 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 4 ML. 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 magnetoresistivity 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 magnetoresistivity of thin Pb films is dominated by superconductivity and weak localization up to 10 T. This temperature is far from the critical temperature of the bulk (7.5 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 the two different 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 Dorn, Martin Keppep, Eugene Kot, Ulrich Köhler, Ruhr-Universität Bochum, Bochum, GERMANY.

The nucleation and initial growth of iron silicide on Si(11 1 3), Si(5 5 12) and Si(1 1 4) is studies in comparison to Si(111) using high temperature STM. During MBE deposition of iron silicide the precursor Fe(CO)₅ at temperatures up to 600°C directly show the kinetics of the alkyl formation on the surface. Whereas on Si(111) 3D-silicide islands already form in the submonolayer range, a complete wetting layer is formed at all yielders for temperatures below 560°C. A mixture of different periodicities (2x2), with a ranging from 2-6, is found. The closed wetting layer strongly hinders the vertical oxidation 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. 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 eventual crystallization into micron sized grains. 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 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 100 eV 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 diffraction 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 COalesCING EVENTS IN POLYCRYSTALLINE THIN FILMS OBSERVED BY IN SITU TEM-IMAGE 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. Hall, 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 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 coalescing 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 [k01] to [001] as the film grows thicker than 2.5 nm; we attribute this to changes in surface energy associated with the known diffusion of oxygen from the substrate into the first 1.2 nm 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 optimizing grain nucleation and coalescing 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.

230 PM P10.5
KINETIC AND STRAIN-INDUCED GROWTH INSTABILITIES IN Si$_x$ Ge$_y$ EPILAYERS ON VINCINAL Si(001): Christoph Schelling, Guntbert Speck, Peter Schubert, Sibylle Hellmig, Universität Lübeck, Lübeck, AUSTRIA; Markus Subberger, Bert Voigtländer, Institut für Grenzflächenforschung, FZ Jülich, GERMANY.

Compressive in-plane strain was considered to initiate roughening of pseudomorphic SiGe heteroepitaxy through a bunching of steps. Recently, we found (cf. Ref 1) that under growth conditions far from thermal equilibrium, pseudomorphically grown Ge$_x$Si$_{1-x}$ layers developed kinetic 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 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 magnitude and period. On this base we systematically studied the morphology of strained Si$_x$Ge$_{1-x}$ layers deposited either under kinetically limited, or under equilibrium growth conditions. By increasing the composition from x = 0.05 to x = 0.35 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 unit-cell 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, 955 (1999).

2:45 PM P10.6
LATERAL SELF-ORGANIZATION OF Si QUANTUM DOTS BY PERIODIC SUBSURFACE DISLOCATIONS ARRAYS. Franck Fournel, Karine Roussaz, Joel Emery, Jean Luco Rouviere, Denis Buturla, Noeller, CEA-Grenoble, LETI/DEPT. Microtechnology; Thierry Barzin, INSAS-Lyon, Lab. Phys. de la Matière; Pierre Mar, Francis Martin, Marie-Noelle Serenac, 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 μm 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 edge dislocations 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 governs the formation of the self-assembled film, which will control the nucleation process. STM images shows that self-assembled nanocrystals deposited on such template forms 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, 2780 (1999) and A. Boureuet -Surface Science 432, 37, 1999 that analyse the influence of buried stressors on surface energy. This technique of lateral self-organization should have all the requirements for a large scale integration of ordered nanostructures in terms of size, dispersion and density.

3:30 PM P10.7
NON-LINEAR GRINFIELD INSTABILITY OBSERVED IN MULTILAYERED SI(001) STRUCTURES. Wen-Chih Wei, Yung-Jong 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 counteracted by surface tension that prevents short wavelength deformation. This is so-called Grinfeld instability. Non-linear analysis indicates treich formation, and it has been substantiated that fracture and coherent microcrack 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 bilayers of Ge/Si(001) (~1nm/30nm) were grown at 760°C and 540°C respectively. The uncoupled samples were terminated at Ge layers. We found that 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 atomic force microscopy (AFM). Surprisingly, the depths of trenches in (2) extend to over ~30nm. That is, they penetrate deep into the Ge spacer. This contradicts the general thought that trend growth should be effectively limited as it approaches a substrate or interface because the local stress field at the trench tip reverses sign. Furthermore, the ~30nm wavelength of the trench pattern is unexpectedly long. Cross-sectional TEM was also used to corroborate the surface information obtained by AFM. We found sample (1) was mostly elastically strained with partial misfit dislocations. Sample (2) was similar to (1) except that we observed formation of novel vertically aligned 'inveter dot' beneath the Ge layers. Sample (3) was heavily relaxed due to misfit dislocations. This suggests that the non-linear Grinfeld instability plays a role in 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 Nemani, 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 Si$_x$(0.7)Ge$_{(0.3)}$ to 100nm thick by solid source MBE on substrates with surface orientations rotated from [001] to [111] by angles of θ = (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 hex-like structures at 0 degrees to large meso-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 linear along growth features, and the layers vary continuously with the angle of rotation of the substrate. The state of relaxation of each layer is quantified by Raman spectroscopy so that the 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 Si(111) SURFACES. Ingo-Shoung Huang, Mon-Shi Ho, Tien T. Tsong, Institute of Physics, Academia Sinica, Nankang, Taipei, TAIWAN ROC.

A special type of Si magic clusters on Si(111) surfaces are found with a variable temperature scanning tunneling microscopy (STM). They play an important role in mass transport phenomena, step fluctuations, and epilayer growth. We characterize the structure of these clusters and derive parameters using hopping transition rate theory, and Arrhenius analysis [1]. Interestingly, when a Si magic cluster hops out of a 7x7 halfcell, it usually reappears at a site a few hundred A away. The most interesting behavior seen in the long hops of Si magic clusters is that the clusters have a high (65%) migration 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 the corner as well as the preferential detachment of Si magic clusters from Si hillock island edges near the cathode side. As the electronic fields we apply (on the order of 1-10 V/cm) are very small, the strong tendency for these bimodal phenomena is very surprising [2]. [1] I.-S. Huang, M.-S. Ho, and T.T. Tsong, PRL, 83, 120 (1999); [2] M.-S. Ho, I.-S. Huang, 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-ASSISTED STACKING-FAULT STRUCTURES ON LAYER-QUENCHED Si(111) SURFACES. Katsuyoshi Shimada, Tetsuya Ishimaru, Takaharu Watanabe, Tatsuya Yonemitsu, Masashi Osuk1, Tadashi Hoashino and Iwao Oldenbe, 1 School of Science and Engineering, Waseda University, Tokyo, JAPAN; 2 Faculty of Materials Science, Waseda University, Tokyo, JAPAN; 3 Faculty 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 direct-writing-fact (DAW) reconstruction on Si(111) surfaces have been investigated by measuring the time evolution of DAW domain size distribution at four temperatures ranging 360-440°C. The experiments were performed using a scanning tunneling microscope (STM). The growth structures appearing over the whole surface maintained at high temperature were destructed by a non-
second-pulsed laser irradiation. After keeping the specimen in growth temperature, the surface was quenched to room temperature and numerous STM images were obtained in order to extract the size distribution of DAW domain. The experimental results clearly show that the higher the substrate temperature is, the faster the DAW domain growth. The whole process 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 DAW reconstruction is quite rapid. The density of the voids is in the same order as that of the DAW domains formed initially, which suggests that the DAW reconstruction is promoted around the voids. At the next stage, after the disappearance of the voids, the DAW 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 DAW domains nucleate and grow steadily at each temperature. The activation energies for the formation and the annihilation of the DAW structure have been estimated to be 1.62±0.4 and 2.1±0.6 eV, respectively. The difference in the two activation energies reflects the stabilization of DAW domain upon growth.

4:30 PM P10.11


We have been successful in producing arrays of mesa 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 etching method. The present work 'inverts' the previous process by using a pattern of trenches to define the mesa and then depositing Si to grow the atomic steps off the edges. The mesas are created on Si wafers, which are ∼0.5° from the (111) plane by lithography and an ion etching step. 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 temperatures. The minimum 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 rows of monoatomic 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. Finnem and Y. Homma, NTT Basic Research Laboratories, Atsugi, JAPAN.

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 in situ using electron microscope. For specific growth conditions and steps. In 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 granular and substrate, terrace widths play an essential role in the instability. Given the observed crystalline symmetry of the step width, some elaboration to the elementary theory is required. [1] G.S. Brace and A. Zangwill, Phys. Rev. B 41 (1990) 5600 [2] P. Finnem and Y. Homma, Phys. Rev. Lett., to be published [3] Y. Homma and P. Finnem, 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)
P11.4
STUDY OF NUCLEATION PROCESSES DURING ION-ASSISTED MBE GROWTH OF Ge ON Si SURFACES.
Jiro Misu, Toshiro Seki, Gikun H. Takacs; Ion Beam Engineering
Experimental Laboratory, Kyoto University, Kyoto, JAPAN; Iwao
Yamada, Laboratory for Advanced Materials Processing 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 each stage of film formation have been
investigated. The single ion impact traces whose diameters were about
20 nm were clearly observed with atomic resolution on the Si(111) 7×7
surface irradiated with Xe ions. After ion bombardment, vacancies
created in subsurface by the impact start to diffuse towards
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 an 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 a step
edges when the surface with the Ge islands was irradiated by Xe ions
at dose of below 10^6 ions/cm². Number of vacancies is less than the
number of Ge atoms. When the dose was above 10^6 ions/cm², Ge
islands disappearance and the surface morphology was completely
changed. Growth kinetics modified with ion irradiation will be
discussed.

P11.5
POLYCRYSTALLINE Sİ₁₋ₓ Geₓ LAYER GROWN BY THE
UHV-CVD AND UHV-ECR/CVD. Jin-Won Park, Hwan-Kuk Yuh,
Seong-Hyun Lim, Jong Ho Lee, Edson V. Teo, School of MBE,
Seoul National University, Seoul, KOREA; Jong-Ho Lee, Electrical
Engineering, Wookwang University, Iksan, KOREA.

Poly crystalline Si₁₋ₓ Geₓ films are a promising alternative to
conventional polycrystalline Si film for various 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 poly crystalline
Si₁₋ₓ Geₓ films by ultrahigh vacuum chemical vapor deposition
(UHV-CVD) and ultrahigh vacuum electron cyclotron resonance
chemical vapor deposition (UHV-ECR/CVD). Poly crystalline
Si₁₋ₓ Geₓ 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 10-150 nm thick with a rough surface. On the other hand, two
minimirs of GeH₄ pretreatment made the poly crystalline Si₁₋ₓ Geₓ layer continuous and smooth at the same
growth conditions. It is speculated that the GeOₓ layer was desorbed from the oxide surface during the pretreatment, consequently the surface became Ge-rich, which leads to the high nucleation rate of SiGe nuclei.
This new growth technique may help us overcome the difficulty of
poly crystalline Si₁₋ₓ Geₓ 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-ECR/CVD 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, SCHWEIZ.

Fully relaxed, linearly graded Si₁₋ₓ Geₓ buffers with x between 0.5 and 0.7 serve as virtual substrates for thin, coherent Ge-rich channels (up to 10 μm thick) for p-MOS devices.

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/h. The typical layer thickness was 25 μm for X = 0.5 and 10 μm for X = 0.7.

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 SiGe layers were deposited on top of the virtual substrates at temperatures below 500°C and using lower plasma densities in order to suppress strain-induced surface

P11.7
Ge SEGREGATION IN THICK STRAINED SiGe/Si[001] FILMS
GROWN AT HIGH RATES. Matthias Kummer, Hans von Känel,
Laboratorium für Festkörperphysik, ETHZ, ZURICH, SCHWEIZ;
Enver Kh. Makhmudov, Shamilov’s Institute of Crystallography, Moscow, RUSSIA; Alex Dommann, Institut für
Mikrosystemtechnik, NTB, Buchs, SCHWEIZ.

Strained epitaxial Si₁₋ₓ Geₓ 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 of 5 μm and 20 μm, with final Ge concentrations between 2% and 5.5%. High resolution x-ray diffraction (HRXRD) has been employed to investigate the actual composition and structural quality of these films. It turns out that the growth rates of growth rates between 1 and 2 μm/minute. In the case of 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. This segregation can be efficiently suppressed by using additional H₂ acting as a surfactant during growth.

P11.8
RAMAN SPECTROSCOPIC STUDY OF STRESS AND DISORDER
IN SURFACANT-MEDIATED MBE GROWN Ge[211]/Si[211].
G. Price, S. Tari, S. Srinivasan, Univ of Illinois at Chicago, Physics
Department, Chicago, IL; Y. Gogotsi, Univ of Illinois at Chicago, Dept
of Mechanical Engineering, Chicago, IL.

Ge growth on Si in the Stranks-Krstic slow growth mode (2D-3D)
because of the 4.2% lattice mismatch of Ge to Si. In contrast, the faster
geometric growth mode can be altered by surfactant layer deposition in
the [211] orientation. These results suggest that a general stress difference between the two growth modes will be presented describing the differences between surfactant mediated growth in the [211] and [001] orientations.

P11.9
OPTICAL PROPERTIES OF SELF-ORGANISED Si₅ₓGeₓ AND
Si₅ₓGeₓ-MBE Ge NANOSTRUCTURES GROWN ON SiGe TEMPLATE
LAYERS ON Si [118]. G. Bremond, P. Ferrandis, A. Souff, INSa de
Lyon, Laboratoire de Physique des Surfaces, Villeurbanne, FRANCE; M. Abdallah, A. Renda, I. Berberian, CNRS,
Centre de Recherche sur les Mecanismes 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 [Ge₅ₓSi₁₋ₓGe₅ₙ] deposited on Si substrates realized by gas source MBE (GS-MBE) and solid source MBE (SS-MBE). The process used consists in realizing in a first step a Si₁₋ₓGeₓ template layer with a "self-patterned" morphology. Such patterning, based on periodic morphological modulation of the surface is used to define and organize the Ge nucleation 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 dot deposition on the template layer. This is followed by a short period of growth from the 2D material, which is then grown to a thickness of 3 ML. This case of n = 3 ML has been found to be more intense in GS-MBE thanks to the partitioning rule of the hydrogen atoms. The 2D to 3D growth transition is accompanied by the occurrence of a red-shifted indirect band (L) which becomes dominant at higher temperatures. This transition is obtained from dots directly deposited on Si substrate, narrower band is obtained from dots deposited on the template layer. Moreover

the redshift 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 formation of the device bands while show similar optical and structural properties in both growth techniques. The main difference between GS-MBE and SS-MBE concerns a lower energy shift in the PL of the SS/SS/SS Ge dots that we shall discuss in the next section 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; Seo-Min Lee, Seo-Ho Lee, Ah-Soo Lee, KOREA; Young-Ho Lee, Soo-Kyun Park, Duowoo Electronics Co., Ltd., Seoul, KOREA.

SiGe selective epitaxial growth (SEG) technique has been widely studied and employed for the layer-by-layer deposition of semiconductor heterostructures, including high performance 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 nodulation formation on the mask area. Also, any possible changes in adsorption diffusion characteristics would affect the SEG characteristics.

In this paper, 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, SiH4, Cl2, GeH4 and HCl gas-mixtures as source gases. The growth temperature varied from 750 to 770 °C and a pressure was fixed at 40 Torr. Scanning electron microscopy (SEM) and Nomarski interference microscopy 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 nodules (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 adsorption 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. Remedios1, 2, 3, Ethamhos Kaur1, 2 and P.C. Koleske1 2 Department of Physics and Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA. 1, 2 Physics Department, University of Crete, Heraklion, 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 Bi-tipped SiGeC alloy has been very recently manufactured. The different physical and chemical traits of this system, in contrast with the native of the Si(100) surface, give rise to several interesting phenomena. C incorporates into the Si lattice because of the enhanced surface stability, despite its bulk solubility is of the order of 10-4: the surface reconstruction changes from (2x1) or (2x2) to a (4x4) periodicity; in contradiction to the empirical rule that the most electronegative atoms prefer to be located at surfaces. This system seems to transform into a surface state with the atomic 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 quantum chemical 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.


Explosive crystallization of germanium exhibits three distinct kinetic and morphological regimes. Dynamics of the growth processes, and the resulting morphologies, have been here examined in detail. Analysis 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 the morphology consisting of a way 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 generally low average crystallization velocities, suggest a kinetic instability that leads to staggered motion of the crystallization front. At high temperatures the velocity saturates at around 1.5 m/s. The morphologoy consists of columnar-like structures with surface features extending perpendicular to the growth front. Long needle shaped single crystall grains form in this nearly unidirectional pattern. This regime arises from self-selection of a stable, high velocity, growth mode. At intermediate temperatures this regime 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.


Strain distribution control on the Si wafer scale is an important goal because it enables the fabrication and selective positioning of nanostructures. We demonstrate an amorphous silicon film formation 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 an annealing in an Ar atmosphere containing 2% O2 at 1350 °C for 2.5 hours. The volume distribution 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 200 nm below the surface. At an implantation density of 5 x 1017 cm-2 the (001) wafer surface is free of defects due to the buried oxide, whereas a few line defects are observed on 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), doses ±10 nm high form, allowing the implantation defects to be etched from the surface. The surface is also investigated following 100 nm Si homoepitaxial growth, using AFM and micro-Raman spectroscopy. During growth, RHEED confirmed film-substrate coherence. AFM demonstrated that the height of the surface topology 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 MECHANISMS AND DEFECT FORMATION. T. Motoki and K. Nishiyama, 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 65.24x65.24x43.4 A^3 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 small facets in the [001] pulling, while it was smooth in the [111] surface in the [111] pulling. [2] The melt growth in the [001] direction was directly occurring 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 nucleus was first created and then followed by double-layer growth; and [3] defect formation was initiated by a Smember 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 x>1111 reconstruction. Examples of atomic motion at the solid/liquid interfaces during the melt growth obtained by MD simulations described above will be shown in a movie.

P11.15
Abstract Withdrawn.

P11.16
ORDERING IN AlGaN: THERMODYNAMICAL AND X-RAY ANALYSIS S. Rufforth-Cher, O. Briot, M. Moret, R.L. Aldumend, GE, Universe Montpellier II, Montpellier, FRANCE.

Up to date, different groups have reported ordering phenomena in nitrides alloys like InGaAs 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 each system using the Kesting 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 has 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 1% steps, in the full range of composition from GaN to AlN. All the growth parameters were kept constant except for the Al 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

The ratio between the Group V and Group III flux (the V/H 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 group-III nitrides, 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/H ratio. A new method, utilizing 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/H ratio across a large part of a rotating sample.

P11.18
INTERFACIAL ROUGHENING IN GaAs/GaSb 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: 0.003%) GaSb-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 GaSb-GaAs interfaces show irregular roughening on both micron and atomic level. (113) faceted roughening occurs in the GaAs2-GaSb interfaces, leading to the formation of V-shaped grooves. For GaSb2 layers exhibiting atomic-scale roughening, the number of dislocations, mostly (114)-type and in a dipole configuration, are confined in a zone of about 0.12 nm width along the interface, and dislocations are rarely observed deep inside the layers. For GaSb2 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 GaSb2 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. Jeongsik Yoong, Dept. of Physics, MIT and Gordon McKay Laboratory of Applied Science, Harvard University, Cambridge, MA; Yi-Jun Chiu, Electrical and Computer Engineering Department, 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 Al. A cap 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 plan 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 peak. The temperature dependence of the main 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 nanostructure.

P11.20
DYNAMICS OF Ga CLUSTERS ON GaAs (001) SURFACE. Shiro Tsukamoto, Nobuyuki Koguchi, National Research Institute for Metals, Tsukuba, JAPAN.

Dynamics of Ga clusters on a GaAs (001) surface were successfully observed by scanning tunneling microscopy (STM) and molecular beam epitaxy (MBE) were equipped with not separated each chambers but one incorporated unit. With the substrate temperature of 290°C, reaction 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^-10 torr. Ga tip emitter clusters[4] moved along the missing dimer row of the (2x4)/2 surface with keeping its shape and become decorated Ga atoms were stepped back-step edges and moved to the most active sites. Moreover, with the substrate temperature of 528°C, RHEED pattern showed a (4x2) Ga-stabilized surface reconstruction[4] 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] T. Tsukamoto and N. Koguchi, J. Cryst. Growth 201/202 (1999) 118. 2] T. Tsukamoto and N. Koguchi, J. Cryst. Growth 289 (2000) 258. 3] T. Tsukamoto and N. Koguchi, Jpn. J. Appl. Phys. 33 (1994) L1165. 4] J. Cryst. Growth 150(1995) 33.

P11.21
INITIAL GROWTH OF EPITAXIAL ZnO ON a-SAPPHIRE. Paul A. Furst, K. Iwata, K. Nakamura, A. Yamada, K. Misakura, and S. Niki, Electrotechnical Laboratory, Tsukuba, JAPAN, K. Nakamura, T. Tsuha, H. Takasu, Rohm Corporation Kyoto, JAPAN.

High quality, c-oriented ZnO epitaxial films have been grown on the surface of sapphire using molecular beam epitaxy. The use of a nitride substrate has been shown to eliminate rotational domains and related structural defects present in ZnO grown on sapphire which 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 (HRRSM), and EXAFS data to elucidate on the growth mechanisms active during the initial growth process. ZnO films were grown by molecular beam epitaxy onto c-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, 45, 60, and 800 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][0001] for growth times of 45 s or more, while no in-plane orientation could be seen with experimental error for growth times of 30 s or less. In contrast, HRRSM along the surface normal indicated the the presence of a narrow mosaic (~10 arcsec) with a preferential orthogonal graphite with a distribution of lattice constants from ~0.5 nm to 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 Ga/In/Cd \textit{HETEROFUNCTIONS}. Paul Bokros1, Robert Spoerke2, Yue Xing1, N-D. Browning1, S. Sinnoitham1, Microphysics Laboratory, University of Illinois at Chicago, Chicago, Physics Department, Illinois, 1Facultes Universitaires Notre-Dame de In Paix, Laboratoire
Interdisciplinaire de Spectroscopie Electronique, Namur, BELGIUM.

Growth of single crystal wurtzite Cadmium Sulphide on CdTe[111]B substrates has been achieved using molecular beam epitaxy. Cadmium Sulphide is a wide band gap semiconductor with Eg = 2.42 eV, used mostly as window material for high efficiency solar cells, in tandem with CdTe and CdTeF2 alloyed layers. Other potential 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 alloy, suitable for measuring optical frequency difference. These two important groups of growth methods for CdS have had their focus on the zinc-blende structure. However, the wurtzite structure is the thermodynamically stable phase. In this work, we report the growth of CdS on CdTe[111]B/112 substrates. Cadmium Sulphide can be doped n-type whereas p-type is very difficult due to strong self-compensation. During the growth, an insitu dopant reflection high energy electron diffraction (RHEED) pattern is used in several hundred nanometers with the molybdenum X-ray diffraction crystal orientation line. The epitaxy was grown by high-temperature, high-quality, high-temperature 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 layer. Based on Vegard’s law, the shift in the XRD scans 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.

Peter A. Schier, Thomas M. Klauk, Michael Becker, Horst P. Strunk, Institute for Microcharacterization, Friedrich-Alexander-University Erlangen-Nuremberg, GERMANY; Frank Schroeder, Manfred Neudeck, Department of Experimental Physics I, University of Hamburg, GERMANY.

The effect of substrate misorientation on the incorporation of defects during molecular beam epitaxial (MBE) growth of GaAs at reduced substrate temperature (LT-GaAs) has been studied. The presence of excess epitaxial layers grown on GaAs(100) substrates, exactly oriented and tilted up to 10° towards the [111]B 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 by 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. Chooop, B.P. Sharma, and T. Venkatesan. Center for Solid State Devices, University of Maryland, College Park, MD, 1 also with Electrical and Computer Engineering Dept., University 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 248 nm KrF excimer laser was varied from 1.0 to 2.5 J/cm² while the substrate temperature and oxygen pressure were fixed at 750°C and 1 x 10⁻³ Torr, respectively, which were optimized previously [1-4]. The deposited ZnO epilayers have been characterized by x-ray diffraction (XRD), electron microscopy and atomic force microscopy (AFM) and x-ray diffraction (XRD) analysis. XRD analysis shows that ZnO films deposited with low laser fluence have hexagonal hillocks while the surface becomes inhomogeneous at higher laser energy density. High quality x-ray diffraction patterns show that ZnO films deposited with low laser fluence have a (0001) orientation. The film thickness and substrate temperature, the fractal dimensions of the films were determined to increase from less than 1.06 being approximately the value of the film-thickness-limited roughness to 1.88 and eventually up to a value of 2.0, which corresponded to a uniform ZnO layer with fines growth in the electronic devices. Mode.

P12.1
DIMER VACANCY LINE DEFECTS ON Si(100) 2x1 SURFACE. Eunja Kim and Chang-feng Chen, Department 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 images, we used a very large supercell [32x2], so that the interaction between one DVL and other DVLs 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 DVLs instead of each accumulating at one place forming a crystal of four individual single DVLs. This tendency remains even at higher densities of 0.30 ML and 0.375 ML. It seems that introducing more DVLs does not induce larger DVLs with wider widths, but rather more interactions between DVLs. The experimentally suggested model of dimer line defect, [21], is energetically favorable to the DVL model.

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. MROEK, H.P. STRUNK, Institute for Microcharacterization, Friedrich-Alexander-University Erlangen-Nuremberg, GERMANY.

GaAs epitaxial layers are grown from Ga-source onto spherical-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) and atomic force microscopy (AFM). Selected areas are investigated by reflection electron microscopy (REM).

In the region around the exact 001 orientation (± 0.1 degree) a very smooth facet develops containing monosteps only. This tendency induces 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 steps in height. We find in both, facet and terrace region that the emergence points of dislocations block the lateral motion of growth steps. This leads in the terrace region to formation of pronounced depressions elongated in the lateral growth direction, that are reminiscent of telluriums. 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. T. 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 arc ion source. The fractal dimension of the patterns was found to correlate with the temperature rise of the Si substrate, which was evidenced by the implanted Ni ion beam. With increasing the substrate temperature, the fractal dimensions were determined to increase from less than 1.06 being approximately the value of cluster diffusion-limited aggregates (DLA) to 1.88 and eventually up to a value of 2.0, which corresponded to a uniform NiSi₂ layer with fines grains applicable in the electronic devices. Meanwhile, a pre-deposited Ni layer on the Si surface was found to have some influence on the growth of the fractal patterns. By increasing the thickness of the Ni overlayer, the fractal dimension increased a little, yet the
characteristic of the corresponding pattern did not change. In addition, the measured sheet resistance of the Si surface varied in a well controlled manner in accordance with 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 wafer as well as the interactions among the Ni and Si atoms or 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

P1.13.04 DIFFUSION AND REACTION KINETICS OF NIOBIUM/GOLD THIN FILMS FOR FIRST LEVEL DEVICE INTERCONNECTS.
Robert Foster, Avis 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.

P1.13.05 TIN/GaAs THIN FILM STRUCTURES FOR GATE METALLIZATIONS.
Chichang Zhang, Avis Christou, Dept. of Materials Science and Engineering, Univ. of Maryland, College Park, MD.

The shape memory alloy TIN 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 TIN compositions were deposited by electron beam deposited on GaAs initially as thin layers of Tl and Ni. The intermetallic phase of TIN was formed by annealing and completely intermixing the multilayers at 370°C. The intermetallic phases were investigated by 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 MESFET's with TIN 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.

P1.13.06 IMPROVEMENT OF THIN PALLADIUM SILICIDE FILMS ON (100) SILICON SUBSTRATES BY INCORPORATING PHOSPHORUS DOPANT.
Ming-Hsien Jiang, Chin-I Ouyang, National Taiwan University and National Taiwan Institute of Science and Technology, Dept. of Electronic Engineering, Taipei, TAIWAN; Huang-Cheng Cheng, Cheng-Tung Lin, National Chiao-Tung University, Dept. of Electronic Engineering, Hsin-Chiu, 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 junctions. However, diffusion 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 BF$_2$ dopant into thin Pd films deposited on Si substrates and then annealing, the thermal stability of thin Pd$_x$Si$_{1-x}$ films can be improved relative to the control samples without dopant incorporation. The degree of improvement is affected by the fluorne concentration around the silicide/Si interface and thus the BF$_2$ implantation energy. On the other hand, as for the samples formed by implanting phosphorus dopant into thin Pd films and then annealing, the thermal stability and the silicide conductivity of thin Pd$_x$Si$_{1-x}$ films can be significantly enhanced. The control samples show a large increase of sheet resistance from about 10 kOhm/sq. to about 250 kOhm/sq. as the annealing temperature is raised from 600 to 700°C.

P1.13.07 SURFACTANT MEDIATED GROWTH OF MnSi$_x$ ON Si[001].
S. Tschmel, H. Hornsbach, A. Mogilniensk, M. Falke, G. Bednorz, H.-J. Hennberg, University of Technology, Chemnitz, GERMANY.

Surfactant mediated film growth has drawn extensive attention since the pioneering works in the system Si/Ga. 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$_x$, 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 electronic ground state 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 sample surface, 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 enhances 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 Si(001) surface and for the co-deposition of Mn and Sb on Si[001]. A residual Sb coverage close to one monolayer at the sample surface has been determined for both the preparation conditions. The variation of Sb coverage from 0 to about 1 ML (1 ML = 6.78x10$^{14}$ atoms cm$^{-2}$) of the Si[001] surface before deposition of Mn allows a scaling of the island density over two orders of magnitudes.

P1.13.08 EPITAXIAL IRIDIUM FILM GROWTH ON STRONTIUM TITANATE.
Z. Dai, A.P. Liu, C. Bednarski, and B. Goldberg, Center for Sensor Materials and Department of Physics & Astronomy, Michigan State University.

Epitaxial (100) iridium films have been successfully grown on (100) SrTiO$_3$ (STO) substrates via UHV electron beam evaporation. The epitaxial relationship between iridium films and STO substrates, as determined by RBS (Rutherford Backscattering Spectroscopy)/Channeling, is Ir(100)/STO(100). Ir(110)/STO(110), and Ir(111)/STO(111). Our best epitaxial Ir films are characterized by small Ir(208) rocking curve FWHM (full width at half maximum) < 0.8°, smooth surface 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 in the film thickness increases up to 500 nm. We have found that the crystalline films can be obtained on Si 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. Charke, Department of Physics, University of Michigan.

We have shown recently that it is possible to achieve dramatic smoothing of epitaxial Cu (001) oriented films grown on nitrogen terminated Si(111) surfaces, through the use of temperature range below significant sputter formation at the surface (350 K < T < 45K). [1] We found in this temperature interval a lower activation energy (0.4 to 0.3 eV) than the reported value of 1.1 eV for (001) Copper in the temperature range 330 K < T < 380 K. [3] In order to clarify the mechanism of sputter smoothing, 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 specific temperature on the surface, leads to improved film roughness despite the somewhat high high activation energy (1.2eV) measured for mass transport. Our findings also indicate that the presence of a dramatic smoothing when annealing the [111] Cu films, as compared with wafer. For reported behavior (001) Cu films grown on H-terminated (001) Silicon is related to lack of H-termination on the Cu-Si interface. [1]. R.A. Lukaszew, Y. Sheng, C. Uher and R. Charke, Appl. Phys. Lett. 76, 724 (2000).


P11.37

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-grain 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-μm-wide Cu lines, created from the blanket films by standard lithography techniques, are subject to electromigration tests at constant current densities of 1.5×15 MA/cm² in an Ar ambient at temperatures between 150 and 400°C. The time to failure of high 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 CaF₂/Si(111). Y.V. Schuster, M.L. Yakovlev, L.J. Schowalter, Rensselaer Polytechnic Institute, Department of Physics, Troy NY; K. Doidenko, 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 CaF₂/Si(111). The films allow to insulate the metal from the silicon for electrical characterization. Reflection high energy electron diffraction (RHEED) indicated that the Al films grew epitaxially in 111 orientation despite the large (∼29%) lattice mismatch. Most of the Al appears to grow in the same orthorhombic orientation as CaF₂ 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 proceeds through formation of 3-dimensional islands that then coalesce as the thickness increases. Using an Al deposition rate above 1 nm/s at room temperature, we were able to obtain continuous films as thin as 10 nm with roughness less than 2nm, as measured by atomic force microscopy. Scanning tunneling microscopy reveals internal structure of them originating at screw dislocations. The density of these dislocations was around 10¹⁷/cm². Measurements of the Al resistivity as a function of film thickness showed a clear size effect below about 3nm. The Cu was polycrystalline when deposited directly on CaF₂, but grew epitaxially on 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 is 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 3D-domains disappeared, the surface became considerably smoother, and no polycrystalline material formed even beyond 200nm thickness.

P11.39

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 electrodeposited Cu films were deposited on SiN coated silicon substrates with and without Ta or TaN barrier layers. The films were made into membranes by selective photolithographic etching of the silicon with hot KOH to form rectangular 2×10×0.4 mm membranes. The mechanical properties of the composite membranes were investigated using two techniques: 1) resonant frequency measurements performed in vacuum were used to determine the initial tensile stress, and 2) capacitive measurement of bulge height vs argon gas pressure were used to determine the stress-strain behavior. For example, in 1 mm thick Cu sputtered films the lowest resonant frequency membrane 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 was observed by a yield stress increase of about 100 MPa. Creep was measurable with high instrumental stability at applied stresses between 200 and 400 MPa over many hours with a strain rate sensitivity ∆S<3×10⁻⁷. 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 REFRUCTORY 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 scattering probe microscopy (SPM). Aperiodic RHEED 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 smoothing at these thicknesses; growth of 110.1 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. Moreover, at the coverage 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 structure of the materials involved.

P11.41
KINETICS OF GRAIN COARSENING IN GOLD THIN FILMS WITH THE MAZED BICRYSTAL STRUCTURE. Tamar Kadish1, Urlich 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 analyses show a strong dependence of grain growth 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
Spatial variations in the alloy composition of ternary and quaternary III-V semiconductor alloys can result from phase separation or strain. Both macroscopic 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 GaAs$_{1-x}$In$_x$As$_{1-y}$Sb$_{y}$ (0 < x < 0.2, 0 < y < 0.45) is reported. The alloys have a large miscibility gap, but still can exhibit excellent materials properties, and high-performance thermoelectric devices have been developed. Normally lattice matched layers are grown by organometallic vapor phase epitaxy on (001) GaAs substrates with misfit of 0.2% toward (111)A, (100), or (110). 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 spontaneous nucleation of a regular interfacial structure is observed for a wide range of substrate misfits, 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 reciprocal lattice plane and spacing of the interfacial structure. It is found that the crystal structure of the interfacial layers (111)-oriented with increasing film thickness from 60 nm to 1000 nm is a high-symmetry phase. The 6.1 A family of compound semiconductors, InAs, GaSb, and AlSb, provides the basis for a wide variety of novel device configurations. In order to efficiently fabricate high-quality devices, it is critical to understand, characterize, and ultimately control the complex interplay between kinetics and thermodynamics that occur 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 A 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 InSb, GaSb, and AlSb reconstructions exist within the range of typical device growth conditions, this roughening can occur even during homoeptaxy, 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 (Ga1-x)Al$_x$As-like bonds, and discuss how exchange reactions depend on growth temperature and group V species (e.g., As$_2$ vs. As$_4$). Supported by DARPA and ONR.

9:15 AM P12.4
IN SITU OBSERVATION OF FACETING OF VINCIAL GaAs(001) INDUCED BY SILICON. S. Brennan, S. Rieth, SLAC, Stanford, CA; G.B. Stephenson, Argonne National Laboratory, Argonne, IL; P.H. Fuchs, AT&T Laboratories, Florham Park, NJ D.W. Kissner, Celot Communications, Inc., Bloomfield, CO; C. Liddell, IBM Research, Yorktown Heights, NY; K.L. Evans-Lutterodt, Lawrence Berkeley Laboratory, Berkeley, CA. 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 organometallic vapor-phase epitaxy (OMVPE). Undoped growth results in ordered monolayer steps. However, after the presence of silicon the step structure 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 silicon-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.

SESSION P12: SEMICONDUCTOR EPITAXY
Chair: Kenste Horn
Friday Morning, December 1, 2000
Room 302 (Hynes)
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. Pelãel, 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. Ongoing studies on the growth of strained heteroepitaxial systems combine a theoretical with experimental approach combining the mechanical properties with the growth rate of the thin films. The results of these studies provide insights into the influence of substrate quality on the growth of strained films.

9:45 AM P12.6
THEORETICAL ISLANDING IN THE InNAs/GaAs EPITAXIAL SYSTEM. Thomas Wohler, Institut für Anorganische Chemie, Universität Bochum, Bochum, GERMANY; Anton G. Cullen, 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 because of the potential device applications of self-assembled quantum dot arrays. However, the mechanisms underlying the island formation transition are still not well understood. The present work focuses on the epitaxial InNAs/GaAs system, with layer deposition by metal-organic vapor deposition. The growth of strained layers during the early stages of growth is examined using transmission electron microscopy and detailed, nanoscale 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.

10:05 AM P12.8
DISLOCATION FORMING IN PbTe HETEROEPITAXY ON PbTe (100) SUBSTRATES. Karin Weisser and Gunther Spriggs, Johannes Kepler Universität, 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 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 <001> directions. From atomically resolved lattice images, the dislocation Burgers vector is found to be 1/2 (001) parallel to the interface. This unusual misfit dislocation configuration is explained by the fact that the easy glide plane is usually 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 relaxation of the dislocation density 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 inter-dislocation spacing of only ±10%, which is much better than the typical 10% 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. Hendrick, O. Malis, J.D. Brock, Cornell University, Ithaca, NV.

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 reaction 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 during the very many minutes of GaN nucleation. We are developing a model for this process based on the finding that ions break apart 2D islands. Related experiments show that only a single monolayer of GaN is needed for the growth of higher quality thin films. These recent x-ray scattering experiments are the first of their kind and demonstrate the feasibility of using these techniques to determine the growth conditions for the first monolayer of GaN on [0001] sapphire.

11:15 AM P12.10
BALLISTIC ELECTRON EMISSION MICROSCOPY ON A SINGLE MONOLAYER Pb/Si(111). I. Akfedor, P. Evans, V. Narayanamurti, J. Golovchenko, Harvard University, Cambridge, MA.

We will discuss the recent realization of an in-situ BEM experiment with epitaxial monolayer of Pb on a 7x7 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 BEM measurements. Experiments were performed in a constant-current mode of STM. With the STM tip above the Pb 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 in a two-dimensional metal layer grown on a semiconductor substrate by Molecular Beam Epitaxy yields a Fermi level nearly flat with a Fermi energy of about -1 eV. This feature can be exploited 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 STS-MD. J.A. Venable, 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 450°C indicates a critical nucleus size of \( i = 3 \). The temperature dependence in the range 300-700°C is well fit by CNT using \( i = 1 \), diffusion energy \( E_d = 1.1 \) eV and island binding energy \( E_b = 0.4 \) eV. These values are not consistent with the direct hopping measurements of Ti-dimer-energies (\( E_d = 1.8 \) eV) reported by Ishiyama et al (Phys. Rev. B51, 1995 p. 2980). 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 INTERACTIONS OF TiSi 2 ON Si SUBSTRATES. R.J. Nemunich 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 in 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.