SYMPOSIUM O

Mechanisms of Surface and Microstructure Evolution in Deposited Films and Film Structures

April 17 – 20, 2001

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of the Materials Research Society
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* Invited paper

SESSION O1: EPITAXIAL GROWTH I
Chairs: Andrew Zangwill and Haydn N.G. Wadley
Tuesday Morning, April 17, 2001
Salon 7 (Marriott)

8:30 AM *O1.1
COARSENING MECHANISMS IN SURFACE MORPHOLOGICAL EVOLUTION. Thomas Michely, I. Physikalisches Institut, RWTH Aachen, Aachen, GERMANY.

Based on a temperature dependent, quantitative STM analysis for homoepitaxial growth and erosion of Pt(111) several atomic scale mechanisms possibly responsible for coarsening of mounds and pits are discussed: (i) noise assisted coarsening, (ii) coalescence coarsening, (iii) step edge diffusion present only during deposition or erosion, (iv) step edge diffusion present even in the absence of deposition or erosion resulting from thermal creation of species being mobile along steps and (v) step atom detachment. For Pt(111) mechanism (iv) - the thermal creation of species being mobile along the steps - is found to be decisive: Only when step adatoms are thermally excited at kinks coarsening takes place. It is argued that for many low index surfaces this coarsening mechanism is likely to be operative. Instead of a surface diffusion current driven by changes in surface curvature frequently assumed in phenomenological theory as origin of coarsening, it appears thus that even at high temperatures coarsening may be driven only by differences in curvature along contours of constant height.

9:00 AM O1.2
HAVE WE FOUND THE FINAL EXPLANATION FOR THE ONSET OF RAPID INTERLAYER MASS TRANSPORT? Margret Giesen, Harald Ibach, Forschungszentrum Juelich, IGV, Juelich, GERMANY.

In previous STM investigations of multilayer Cu island decay on Cu(111) we reported on the observation of a novel rapid interlayer mass transport mechanism [1, 2]. The rapid island decay sets in when island edges in a multilayer island stack approach below a critical distance. For Cu(111), this distance was found to be about 6 densely packed atomic rows independent on temperature. We could also show that the island stack decay could be explained if one assumes that the step edge barrier for interlayer mass transport vanishes if the island edges are closer than 6 atomic rows. As a reason for the vanishing of the step edge barrier we proposed an electronic effect. Assuming that island edges served as impenetrable barrier for electrons we could show that in the case of Cu(111) the surface state would be shifted beyond the Fermi level due to quantum confinement at the critical distance. Rapid island decay is also observed for Ag(111). Here one would expect the critical island edge distance to be about 24 atomic rows at 300K. In addition one would expect this value to be strongly temperature dependent. From recent STM studies, we find, however, that for Ag(111) rapid decay sets in for island edge distances of about 6 atomic rows independent on temperature [3]. We discuss the new results and propose a microscopic mechanism for rapid island decay involving an exchange process at kink sites. [1] M. Giesen, G.S. Icking-Konert, H. Ibach, Phys. Rev. Lett. 80 (1998) 552. [2] M. Giesen, G.S. Icking-Konert, H. Ibach, Phys. Rev. Lett. 82 (1999) 3101. [3] M. Giesen, H. Ibach, Surf. Sci. 464 (2000) L697.

9:15 AM O1.3
RAPID ADATOM ISLAND DECAY ON Cu(111): A KINETIC MONTE CARLO SIMULATION STUDY. Mats I. Larsson, Karlstad University, Karlstad, SWEDEN.

Kinetic Monte Carlo (KMC) simulations are used to investigate the recent scanning tunneling microscopy (STM) measurements of fast decaying adatom islands on Cu(111) performed by Giesen, Schultze Icking-Konert and Ibach [1]. The KMC model is a full diffusion bond-counting model including nearest neighbor as well as second-nearest neighbor interactions. The modeled potential energy barriers are found to correspond well to the experimental ones for the studied temperature range 314 K to 500 K. The investigation consists of two parts. Firstly, reduced activation energies for adatom migration along close-packed step edges are shown to be very important to attain rapid decay of the islands, in accord with the STM measurements. To obtain the best correspondence to the measurements, the 1D Ehrlich-Schwoebel (ES) barrier for adatom hopping around island corners has to be fully suppressed. Secondly, for encounters between steps in adjacent atomic layers of an island it is demonstrated that a moderately reduced activation energy for interlayer adatom transport is enough to obtain correspondence between simulations and experiments, provided that the 1D ES barrier for corner transitions is reduced to zero. The results presented in this report are interesting because they demonstrate that dramatic macroscopic effects can be generated by very small changes of the potential energy barriers that are controlling the surface diffusion rates. [1] M. Giesen, G. Schulze Icking-Konert, and H. Ibach, Phys. Rev. Lett. 80, 552 (1998).

9:30 AM O1.4
TEMPERATURE-DEPENDENCE OF MOUND FORMATION DURING MULTILAYER GROWTH OF Ag/Ag(100) FILMS. K.J. Caspersen, A.R. Layson, C.R. Stoldt, P.A. Thiel, J.W. Evans, Iowa State University, IA.

A current challenge is to characterize the dynamics of mound formation induced by step-edge barriers inhibiting downward transport during multilayer growth of homoepitaxial films. Available experimental data has been limited, often estimating roughening and coarsening exponents for only a single temperature, and being subject to over interpretation. Thus, we have performed a comprehensive VTSTM study of mound formation in the Ag/Ag(100) system between 175K and 300K [1]. Behavior was interpreted using detailed atomistic modeling which precisely describes irreversible island formation in each layer, and incorporates non-uniform step-edge barriers, a realistic treatment of periphery diffusion at island edges, and downward funneling deposition dynamics [2]. All these aspects of the underlying atomistic dynamics are important for a realistic description of mound dynamics in the Ag/Ag(100) system, including such features as the strong temperature-dependence of mound coarsening and slope selection. [1] C.R. Stoldt, K.J. Caspersen, et al., Phys. Rev. Lett. 85 (2000) 800. [2] K.J. Caspersen, C.R. Stoldt, et al., Phys. Rev. B, submitted (September 2000).

9:45 AM O1.5
TEMPERATURE DEPENDENCE OF THE ROUGHENING EXPONENT β FOR THE GROWTH OF Cu ON Cu(001). Cristian E. Botez, William C. Elliott, Paul F. Miceli, University of Missouri-Columbia, Department of Physics and Astronomy, Columbia, MO; Peter W. Stephens, State University of New York, Department of Physics, Stony Brook, NY.

X-ray scattering has been used to study the kinetic roughening of Cu(001) surface during homoepitaxial growth. The coverage dependence of the root-mean-square (rms) roughness, σ, obtained from specular reflectivity data, was measured for temperatures between 160K and 370K. At all temperatures the rms roughness was found to increase as a power law $\sigma=\Theta^{\beta}$, for coverages, Θ, ranging from 3 to 96ML. The roughening exponent, β was observed to depend on the temperature of the substrate: at low temperatures ($T\lesssim 200K$) $\beta\approx 1/2$, while above 200K β monotonically decreases, reaching 1/3 at T=370K. The difference between these results and those of a previous helium-scattering measurement will be discussed.
Support is acknowledged from NSF under contracts (PWS) DMR-9202528 and (PFM, CEB, WCE) DMR-9623827 and MISCON under DOE grant DE-FG02-90ER45427. The SUNY X3 beam line is supported by the DOE, under contract DE-FG02-86ER45231 and the NSLS is supported by the DOE, Division of Material Sciences and Division of Chemical Sciences.

10:30 AM *O1.6
SIMULATING FILM GROWTH WITH ACCELERATED DYNAMICS METHODS. Arthur F. Voter, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM.

A significant problem in the atomistic simulation of film or crystal growth is the time scale limitation of the molecular dynamics (MD) method. In the simulation of vapor deposited growth of a film, MD is ideally suited for describing the individual deposition events, but, being limited to nanoseconds, is hopelessly inadequate for describing the activated diffusion and reorganization events that occur during the milliseconds or seconds before the next atom deposition. To overcome this type of problem, we have been developing accelerated dynamics methods that retain full atomistic, dynamical detail in describing basin-to-basin diffusion events, but which reach much longer time scales than MD. In essence, these methods (hyperdynamics, parallel-replica dynamics and temperature accelerated dynamics) achieve this extension in time scale by sacrificing information about the vibrational dynamics. In particular, we have recently found that the temperature accelerated dynamics method is ideally suited for studying crystal growth at low temperatures (e.g., at roughly 100K and below, where the computational boost can be in the billions). We have begun performing metallic growth simulations at deposition rates in the monolayer/second range, enabling fairly direct comparision with recent surface-science experiments. I will discuss how this is achieved and present our latest results.

11:00 AM O1.7
AN ACCELERATED KINETIC MONTE CARLO METHOD FOR SIMULATION OF THIN FILM DEPOSITION. David G. Goodwin, Division of Engineering and Applied Science, Caltech, Pasadena, CA; Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University, New York, NY.

Kinetic Monte Carlo (KMC) simulations of epitaxial thin film growth can be slow, since the timestep is limited by the fastest events, which

are typically the nearest-neighbor migrations of adatoms on terraces. We present here an accelerated scheme in which adatoms are propagated in single operations over long distances within a terrace, up to the distance to the nearest step. Precomputed solutions of a steady-state diffusion equation in a simple geometry are used to generate the necessary propagation event probabilities. All other events are treated by KMC. In simplest form, the algorithm is valid only in the low adatom density limit, in which each adatom executes an independent random walk until it reaches a step or desorbs. However, by constraing the maximum independent propagation distance appropriately, it may be extended to higher adatom density and even used in the presence of island nucleation. This algorithm is substantially faster than standard KMC when the diffusion length is large. Preliminary numerical comparisons have shown decreases in total simulation time in some cases of more than an order of magnitude.

11:15 AM O1.8
AN INTEGRATED MOLECULAR DYNAMICS AND MONTE CARLO APPROACH TO STUDY EPITAXIAL DEPOSITION OF SILICON. Sweta Somasi, Bamin Khomami, Chemical Engineering Department, Washington University, St. Louis, MO; Ronald Lovett, Department of Chemistry, Washington University, St. Louis, MO.

Epitaxy on wafers deposits a thin layer of high-purity silicon to create a layer with a different doping concentration and to rid the surface of device-killing voids or crystal- originated pits. A complete description of this process would require molecular details of the motion on the surface and modeling of the growing of crystal surface. However, the extremely different time scales of the two processes make it impossible to study them together. Hence, we use an integrated Molecular Dynamics and Monte Carlo approach for this problem. The key steps in the epitaxial growth of high quality single crystals are the adsorption, diffusion and desorption of various species on the crystal surface. As chlorosilanes are the commonly used precursors for this deposition, we have investigated the rates and mechanisms of surface diffusion and deposition of silicon, hydrogen and chlorine adatoms on a plane Si (100) surface and a surface with single-height steps using molecular dynamics simulations. A detailed finite temperature study of these processes was hitherto not feasible with the existing Molecular Dynamic (MD) techniques due to the long time scales involved. We have circumvented this limitation by developing a classical-density functional inspired MD simulation scheme that allows us to calculate the free energy surfaces of various processes. The rate is determined by using simple transition state theory from the Molecular dynamics determined activation barrier and the pre-exponential. In order to simulate the growing of Si (100) crystal, Monte Carlo scheme was used in which larger system sizes and time steps were used. The rates of the essential steps in the growth were determined by molecular dynamics explained previously and Monte Carlo simulations were performed to track the motion of different adatoms on the Si (100) surface and to elucidate the various steps in epitaxial growth of Si (100).

11:30 AM O1.9
ADDITIVE ENHANCED EVOLUTION OF SURFACE NANOSTRUCTURES: COARSENING AND SMOOTHING OF Ag/Ag(100) FILMS. Anthony Layson, Patricia Thiel, Iowa State University, Dept of Chemistry; Jim Evans, Iowa State University, Dept of Mathematics, Ames, IA.

We report the effects of oxygen on the nucleation, and subsequent coarsening, of Ag islands on Ag(100). Both of these processes-nucleation and coarsening-are ultimately controlled by atomic-scale diffusional-processes. These processes, with and without background gases, provide indirect evidence regarding their effect on atomic-scale diffusional processes. These UHV experiments were performed using High-Resolution Low Energy Electron Diffraction and Variable Temperature Scanning Tunneling Microscopy. Submonolayer and multilayer films of Ag were deposited, with the sample held at 250K and simultaneously exposed to the gas of choice, while subsequent coarsening was monitored after evacuation of the gas. Spot profile analysis shows the nucleation of islands is unaffected in the presence of oxygen, but the rate of subsequent coarsening is enhanced. STM reveals that the known coarsening mechanism for Ag/Ag(100), island diffusion/coalescence, has changed. In the presence of oxygen, Ostwald Ripening becomes active and competes with island diffusion/coalescence in the evolution of the surface islands.

11:45 AM O1.10
EFFECT OF Sb ON THE SURFACE MORPHOLOGY OF CLEAN AND Ag-COVERED Ge(100). Lana H. Chan and Eric I. Altman, Department of Chemical Engineering, Yale University, New Haven, CT.

The interaction of Sb with Ge(100) was investigate as a function of substrate temperature and Sb coverage using temperature programmed desorption (TPD), low energy electron diffraction (LEED), ion scattering spectroscopy (ISS), and scanning microscopy (STM). An Sb desorption peak associated with multilayer physical adsorption was observed at 550 K while a second desorption peak at 980 K was attributed to Sb bound to the Ge surface. Four basic types of Sb clusters were identified at 320 K. At 520 K, Sb started to displace Ge in the top layer creating pits at low Sb coverage. As the Sb coverage was increased, both islands and pits were observed. Intermixing between Sb and Ge was found in both the islands and the original surface layer. Intermixing, however, was limited between 520 K and 620 K when the Ge surface was covered with 1 ML or more of Sb, resulting in the smoothest Sb-terminated Ge surfaces. Regardless of how the Sb layer was prepared, annealing at 800 K roughened the surface severely and increased the amount of exposed Ge, even though no Sb desorbed at this temperature. The surface roughening was attributed to the increased surface area enabling Sb-Ge exchange without burying the lower surface tension Sb beneath the surface. Antimony is used as a surfactant to promote the growth of flat Ge films. The results demonstrate, however, that intermixing can lead to the surfactant severely roughening the surface if the growth of the surfactant layer is not carefully controlled. Subsequent growth of Ag on Sb-terminated Ge(100) surface was studied using LEED and STM.

SESSION O2/R2: JOINT SESSION
EPITAXIAL GROWTH II
Chairs: Thomas W. Michely and Arthur F. Voter
Tuesday Afternoon, April 17, 2001
Salon 7 (Marriott)

1:30 PM *O2.1/R2.1
CONVECTIVE STEP-BUNCHING ON CRYSTAL SURFACES. Andrew Zangwill, School of Physics, Georgia Institute of Technology, Atlanta, GA; Navot Israeli, Daniel Kandel, and Michael Schatz.

Recent theoretical work predicts that uniform step-flow growth can be unstable to step-bunching during heteroepitaxial crystal growth. In this talk, I show that step-bunching of this kind can occur via a convective instability. The convective nature of the instability implies a time-evolution for the system (more common in hydrodynamics and plasma physics) that should allow experimenters to discriminate strain-induced bunching from other types of bunching. More significantly perhaps, convective bunching lends itself to external control in a manner that suggests a new approach to nanoscale morphological patterning of crystal surfaces.

2:00 PM O2.2/R2.2
THE DECOMPOSITION OF tBAA ON SILICON FOR COPPER CVD. Che-Chen Chang, Ing-Jye Huang, National Taiwan University, Department of Chemistry, Taipei, TAIWAN, ROC.

Parallel to the shrinkage of feature sizes to 0.18 mm and below in integrated circuit fabrication is the emergence of a class of complexes that may be employed as CVD precursors of copper. Among the copper precursors used, β-diketonate complexes exhibited a high sublimation rate and a low pyrolysis temperature. The present study explores the possibility of using the nonfluorinated t-butylacetato complex of Cu(II) as the precursor. The β-keto ester appears to alter the properties of the metal β-diketonate complex substantially, leading to an improvement on the precursor reactivity. Static secondary ion mass spectrometry studies on the adsorption and decomposition of the ligand, tert-butylacetylacetate (tBAA), on Si(100) show that at low doses, all tBAA molecules dissociate readily upon adsorption on the surface at substrate temperatures as low as -160°C. The dissociation may occur through tBAA bonding via the ester or the diketo oxygen to the surface. The bond scission occurring at the tBuO-CO bond yields isobutene and surface hydroxyl species. In addition, the OC-CCO bond scission induced by tBAA surface bonding mainly via its carboxylic keto oxygen affords acetaldehyde radical, whereas that via the aceto oxygen yields carbon dioxide and isopropenoxy species. Upon acquiring surface hydrogen, an enol-keto conversion takes place for isopropenoxy species to yield acetone, even at low substrate temperature of less than -126°. The aceto oxygen pathway dominates the cleavage of the OC-CCO bond over the carboxylic keto oxygen path. Possible tBAA decomposition mechanisms at high exposures are also discussed.

2:15 PM O2.3/R2.3
RATE-EQUATION APPROACH TO ISLAND CAPTURE-ZONES AND SIZE DISTRIBUTIONS IN SUBMONOLAYER GROWTH. Jacques G. Amar, Univ. of Toledo, Dept. of Physics & Astronomy, Toledo, OH; Mihail N. Popescu, Fereydoon Family, Emory Univ., Dept. of Physics, Atlanta, GA.

We present a quantitative rate-equation approach to irreversible

submonolayer growth on a two-dimensional substrate. Our method explicitly takes into account the existence of a denuded ("capture") zone around every island, the fluctuations in the capture-zone areas, and the correlations between the size of an island and the corresponding average capture zone. The evolution of the capture-zone distributions is described by a set of Voronoi-area evolution equations which are coupled to the usual rate-equations for the island-densities through local rates of monomer capture. The combined set of equations leads to a fully self-consistent calculation of the size- and coverage-dependent capture numbers. The resulting predictions for the capture-zone and capture number distributions are in excellent agreement with experimental results and Monte Carlo simulations. The corresponding island-size distributions and their dependence on coverage and deposition rate are also accurately predicted.

2:30 PM O2.4/R2.4
THEORETICAL ANALYSIS OF THE GROWTH MODE FOR SILVER METALLIC FILMS ON MgO SUBSTRATES. David Fuks, Mater Eng Dept, BGU, Beer-Sheva, ISRAEL; Simon Dorfman, Dept Phys, Technion, Haifa, ISRAEL; Eugene A. Kotomin, MPI, Stuttgart, GERMANY; Yury F. Zhukovskii, Inst Sol St Phys, Univ of Latvia, Riga, LATVIA; A.M. Stoneham, Dept of Phys & Astr, Univ College, London, UNITED KINGDOM.

It is demonstrated how the growth mode of thin metallic films on insulating substrates could be theoretically predicted combining thermodynamic approach and ab initio calculations for low-coveraged ordered metal/insulator interfaces. Theory predicts conditions for monolayer growth via spinodal decomposition, or for metal cluster nucleation-and-growth mode. This is illustrated by calculations for a long-debated Ag film deposition on MgO substrate. Our ab initio calculations predict high mobility of adsorbed Ag atoms on MgO substrate even at low temperatures which stimulates greatly their aggregation.

2:45 PM O2.5/R2.5
THE EVOLUTION OF SURFACE MORPHOLOGY CAN BE DOMINATED BY BULK (NOT SURFACE) PROCESSES. N.C. Bartelt, J.A. Nobel, and K.F. McCarty, Sandia National Laboratories, Livermore, CA.

The processes that control evolution of surface morphology are almost always viewed as occurring in the topmost one or two surface layers. However, in the work reported here we show that the smoothing of the NiAl (110) surface is dominated by direct exchange of bulk defects (vacancies) at the surface steps, not by surface diffusion. This conclusion is reached by measuring the kinetics of island decay using low-energy electron microscopy. Remarkably, the decay rates are constant in time and totally independent of the local environment (e.g., the width of the immediately adjacent terraces or the size of nearby islands). Given this lack of evidence for any surface current between islands of different curvature, we deduce that surface diffusion is not important to the smoothing process. Instead, we unambiguously show that bulk vacancies are responsible for the smoothing by directly measuring the exchange between bulk vacancies and the surface when the sample temperature is changed. Surface steps advance when temperature is increased and recess when temperature is decreased. These changes result from the increase (decrease) in bulk vacancy concentration for a temperature increase (decrease). Remarkably, the size change accompanying a temperature change is always precisely proportional to the perimeter (step length) of the island. Thus, we conclude that the atoms at surface steps undergo direct exchange with bulk vacancies. Since the steps are interacting directly with the bulk, the surface dynamics are independent of the local environment (i.e., step density and curvature). This conclusion is contrary to (current) conventional wisdom. By sinusoidally varying temperature and measuring the phase shift of step motion as a function of frequency, we can also estimate bulk vacancy diffusion constants.
This work was performed under the U.S. Department of Energy contract DE-AC04-94AL85000 and supported by the Office of Basic Energy Sciences-Division of Materials Sciences.

3:30 PM *O2.6/R2.6
EXPLOITING EPITAXY FOR NOVEL MAGNETIC MATERIALS. Roy Clarke, Alejandra Lukaszew, Ctirad Uher, Vladimir Stoica, Yongning Sheng, University of Michigan, Ann Arbor, MI.

Ever since lode stones were first used for navigation nearly a thousand years ago, microstructure has played a key role in the science and application of magnetic materials. The ability to control magnetic properties through a material's microstructure, and now nanostructure, is central to all current magnetics technology from high density recording media to the development of super-strong permanent magnets. The advent of epitaxy as a practical method for producing high quality thin film materials has opened up many new possibilities for novel magnetic structures, extending the range of growth control down to almost the atomic level. This presentation will focus on the use of template epitaxy to achieve well-defined microstructures and nanostructures in magnetic thin films, in many cases leading to materials that have no counterpart in the bulk polycrystalline form. We illustrate the competing effects of magnetocrystalline anisotropy, epitaxial strain and shape anisotropy, drawing on our recent work in the growth of ultrathin cobalt films on Cu-buffered Si (100) wafers. An important feature of this work is the interplay between low-temperature deposition and mass transport kinetics stimulated by carefully controlled annealing processes.

4:00 PM O2.7/R2.7
VACANCIES AND SURFACE MORPHOLOGY DURING LOW TEMPERTAURE HOMOEPITAXY OF METALS. Cristian E. Botez, William C. Elliott, Paul F. Miceli, University of Missouri-Columbia, Department of Physics and Astronomy, Columbia, MO; Peter W. Stephens, State University of New York, Department of Physics, Stony Brook, NY.

X-ray scattering experiments on the homoepitaxial growth of Ag and Cu show that high vacancy concentrations can be acheived during low temperature deposition. A unique aspect of x-ray scattering is the ability to probe the subsurface structure and the surface morphology simultaneously. It is observed that the vacancies, which can attain concentrations on the order of 2% in Ag, extend throughout the thickness of the deposited film. Moreover, the vacancies are found to have a profound effect on the evolving surface morphology for certain surfaces. The effect of vacancies on the surface morphology will be discussed in terms of prior studies of kinetic roughening in these systems.
Support is acknowledged from the NSF under contracts (PWS) DMR-9202528 and (PFM, CEB, WCE) DMR-9623827 and MISCON under DOE grant DE-FG02-90ER45427. The SUNY X3 beam line is supported by the DOE, under contract DE-FG02-86ER45231 and the NSLS is supported by the DOE, Division of Material Sciences and Division of Chemical Sciences.

4:15 PM O2.8/R2.8
CLOSING THE GAP BETWEEN CRYSTAL-GROWTH EXPERIMENTS AND ATOMISTIC MODELS: TEMPERATURE ACCELERATED DYNAMICS SIMULATION OF Ag/Ag(100). F. Montalenti, S. Swaminarayan, M.R. Sorensen, T.C. Germann and A.F. Voter, Los Alamos National Laboratory, Los Alamos, NM.

We investigate the first stages of growth of $Ag/Ag(100)$ at low temperature. By using the temperature accelerated dynamics (TAD) method [1] we are able to extend the standard molecular dynamics time scales by ~ 10 orders of magnitude, so that experimental deposition fluxes are matched. Indeed, we deposit $4ML$ of Ag for a total simulation time of ~ 1 minute. No *a priori* information on the relevant diffusion mechanisms is needed. We show that activated events can play an important role in determining the growing-surface morphology even at temperatures as low as $40\,K$. Two different impinging-atoms momenta are considered: $0.25\,eV$ and $0.025\,eV$. We show that by lowering the momentum, the role of activated diffusion events becomes crucial in causing film smoothness.
[1] M.R. Sørensen and A.F. Voter, J. Chem. Phys. **112**, 9599 (2000).

4:30 PM O2.9/R2.9
STM INVESTIGATION OF ENERGETIC INSERTION DURING DIRECT ION DEPOSITION. J.M. Pomeroy[a], A. Couture[a], J. Jacobsen[b], B.H. Cooper[c], J.P Sethna[a], J.D. Brock[a]. [a]Cornell Center for Materials Research. [b]Currently with Haldor Topsoe A/S, DENMARK. [c]Deceased August 1999.

In a continuing effort to probe the effect of atomic insertions during hyperthermal ion deposition, thin copper films have been deposited on single crystal copper substrates and characterized using a UHV Scanning Tunneling Microscope. At low temperatures, atomic insertions provide a net downhill current that offsets the roughening effect due to uphill "Schwoebel" currents leading to a net smoothing of the surface. Thin films have been grown at several different energies targeted to observe a crossover from insertion driven smoothing to adatom-vacancy dominated roughening. Copper thin films are deposited near 20 eV using a mass selected ion deposition system that allows precise control over the energy of constituent atoms. Experimental observations are compared with a sophisticated Kinetic Monte Carlo and Molecular Dynamics hybrid (KMC-MD) simulation.

4:45 PM O2.10/R2.10
STUDIES OF SURFACE PATTERN ON Si(100) SURFACE AFTER Cu AND Sn DEPOSITION. Qin Hu, Martin Zinke-Allmang, Ian V. Mitchell, University of Western Ontario, Department of Physics and Astronomy, London, Ontario, CANADA.

We report our studies on Si(100) samples with Cu and Sn deposited in an MBE system followed by annealing. Imaging the surface pattern

with AFM and SEM shows that Cu-Sn non-uniform clusters were formed with their shape not sensitive to the order of metal deposition. Changing the relative amount of Cu and Sn a range of varying morphologies were observed. Pyramidal pits were found on the Si(100) surface with Cu-Sn clusters nucleating and growing from those pits. The direction of growth of the pyramidal pits and clusters is $< 100 >$. The late stage growth mechanism of the Cu-Sn clusters differs from that of pure Sn clusters, leading to the discussion of the growth of epitaxial structures.

SESSION O3: POSTER SESSION
Chairs: Jacques G. Amar and M. V. Ramana Murty
Tuesday Evening, April 17, 2001
8:00 PM
Salon 1-7 (Marriott)

O3.1
SIMULATION STUDY OF COPPER CLUSTER DEPOSITION. Jin Chul Kang, Jeong Won Kang, Ho Jung Hwang, Semiconductor Process and Device Laboratory, Dept of Electronic Engineering, Chung-Ang Univ, Seoul, KOREA.

We investigated copper cluster deposition with classical molecular dynamics simulations. We have examined variations of the substrate temperatures, and the number of the disordered atoms during the simulations. We analyzed the properties of copper cluster impacts, such as sticking and sputtering, intermixing, spreading index, surface roughness and film density, as functions of the cluster size, impact angle and initial energy. As the impact angle of the cluster increases, the sputtering ratio increased. In the case of cluster with the same energy per atom, the sputtering ratio and the root mean square (rms) of the surface was proportional to the cluster size. As impact angle increases, the spreading index and intermixing increase. When local area reach melting state on the surface around impact point of an energetic copper cluster during a few ps, intermixing was easily achieved and a good epitaxial film with bulk density was grown.

O3.2
MODELING Cu DIFFUSION INTO Ta BARRIER. Chun-Li Liu, Motorola Advanced Systems Research Laboratory, Mesa, AZ.

Ta has been used as a diffusion barrier for Cu interconnect technologies. As deposited microstructure of Cu seed layer on Ta barrier by sputtering is fine-grained due to the nature of nucleation process. Grain boundaries in the Cu seed layer may have become one of the sources of vacancies for Cu to diffuse cross the Cu/Ta interface into Ta. Another potential source for vacancies is sputtering itself. The kinetic energy of Cu ions for ionized Cu PVD process is typically capable of creating vacancies at Ta surface. In this work, we calculated defect formation and migration energies in Cu and Ta, including Cu migration energy in Ta and Ta migration energy in Cu. The results indicate that with vacancies readily available at the Cu/Ta interface, Cu diffusion into Ta is more rapid compared to Ta diffusion into Cu. The calculated results support previous experimental observations. A brief discussion on how a dopant can be added to the Cu seed layer or the barrier layer to slow down Cu diffusion will also be given.

O3.3
PHOTOACOUSTIC SPECTRA FROM COPPER-PHTHALOCYANINE FILMS ON SILICON WAFER. Masato Ohmukai, Hitoshi Kubota, Yasuo Tsutsumi, Akashi College of Technology, Akashi Hyogo, JAPAN.

Copperphthalocyanine is attractive as an organic material for electronic and optical use. When the material is deposited on silicon, the optical absorption cannot be measured. We then obtained photoacoustic spectra from copperphthalocyanine films deposited on silicon wafers and investigated absorption properties non-destructively.

O3.4
SHAPE AND MICROSTRUCTURE IN ELECTRODEPOSITED COPPER: SUPERCONFORMALLY-FILLED 500 TO 75 NANOMETER FEATURES. Daniel Josell, Thomas Moffat, Daniel Wheeler, John Bonevich, William Huber, Gery Stafford and David Kelly, National Institute of Standards and Technology, Gaithersburg, MD; Andrei Stanishevsky, Institute for Plasma Research, Department of Physics, University of Maryland, College Park, MD.

We identify an electric yields superconformal electrodeposition of copper in trenches ranging from 500 to 90 nm in width (all 500 nm deep), a unique hysteretic response in the current-voltage (i-E) deposition characteristics of the "superfilling" electrolyte, and a 23% decrease of the resistivity of the electrodeposited copper in less than one day at room temperature. Trenches as small as 75 nm wide and 250 nm deep were also filled. Superconformal electrodeposition was obtained using an acid cupric sulfate electrolyte containing chloride (Cl), polyethylene glycol (PEG), and 3-mercapto-1-propanesulfonate (MPSA). In contrast, deposition from additive-free electrolyte, electrolytes containing the binary combinations Cl-PEG or Cl-MPSA, or simply benzotriazole yielded a continuous void within the centers of the trenches. A large hysteresis in the i-E deposition characteristics is associated with the "superfilling" Cl-PEG-MPSA electrolyte and can be utilized to monitor and explore additive efficacy and consumption. Resistivity measurements performed on corresponding blanket films were used to quantify the relationship between the extent of additive incorporation and its influence on microstructural evolution. The films deposited from the "superfilling" Cl-PEG-MPSA electrolyte exhibit room-temperature recrystallization that results in a 23% drop in resistivity within a few hours of deposition. Reduction of void volume formed during conformal deposition from the nonfilling electrolytes through combination of geometrical leveling effect for trenches with sloping sidewalls and more rapid deposition at trench openings is also demonstrated. This is relevant because some studies have used trenches with sloping sidewalls because they were the best materials available. However, it is perhaps of greater interest as an intentional mechanism for obtaining improved filling of trenches and vias, e.g., from electrolytes that do not provide perfect fill but might be desirable for other reasons.

O3.5
A STUDY ON THE UNIQUE CRYSTAL MORPHOLOGY OBSERVED IN THE POLYCRYSTALLINE COPPER CVD PROCESS. Yuneng Chang, Yalian Chen, Kuanhon Chen Lugwha Institute of Technology, Dept. of Chemical Engineering, Guayshan, Taoyuan, Taiwan, R.O.C.

In this presentation, we will show characterization results from copper whisker growth phenomena observed in an atmospheric pressure CVD. This CVD process used copper acetylacetonate, $Cu(C_5H_7O_2)_2$ as precursor, and H_2O vapor as co-reactant, with trace amount of chromium acetylacetonate, $Cr(C_5H_7O_2)_3$, introduced as activating catalyst reagent, at deposition temperatures exceeding 400°C. SEM and XRD observations show that introduction of 0.08 torr of $Cr(C_5H_7O_2)_3$ vapor into depositing chamber, with H_2O pressure above 10 torr, caused deposited polycrystalline Cu(111) and (200) to evolve whisker morphology. The whisker length ranged from 1 to 10 μm, with a surface distribution density of 0.28-3.2whiskers/μm^2. When deposition temperature raised, the length and radius of whisker increased, but surface distribution density decreased. Also, increasing H_2O partial pressure caused the length and radius of whisker to become larger. By applying Arrhenius equation onto whisker growth rate to deposition temperature data, we have performed calculations showing the growth activation energies for whisker in axial direction is 20 kcal/mol, and 12 kcal/mol in radial direction. Based on such data and SEM micrograph observations, vapor-liquid-solid(VLS) model describing controlling mechanisms for film microstructure was proposed. We employed this model to interpret competitive growth for both directions, and tentatively defined the axial direction whisker growth being surface reaction controlled, and radial direction being mass transfer controlled.

O3.6
PLASMA DIAGNOSTICS AND THE EVOLUTION OF A NOVEL TITANIUM NITRIDE DEPOSITION PROCESS. Chris Muratore, John J. Moore, Colorado School of Mines, Advanced Coatings and Surface Engineering Laboratory, Golden CO; J. Alan Rees, Hiden Analytical Ltd. Warrington, UNITED KINGDOM; Dan Carter, Gregory Roche, Advanced Energy Industries, Inc., Fort Collins, CO.

Film deposition processes employing remotely generated plasmas to deliver reactive species to a substrate, such as ion beam assisted deposition (IBAD) or inductively coupled reactive plasma (ICRP) enhanced deposition, are recognized for their ability to increase deposition rates and modify the (micro- and/or lattice) structure of thin film compounds. Manipulation of extrinsic process conditions (e.g., gas flow, source power, etc.) in IBAD and ICRP processes produces measurable changes in intrinsic process conditions such as ion and electron energy distributions and densities. Intrinsic deposition conditions, when correlated to film properties, yield useful information about processing/structure/property relationships. This information continues to change the way we design our deposition processes and equipment. For example, we can measure the reactive ion density and energy distributions of the ICP and ion beam sources. By varying the source gas composition and power conditions it is possible to optimize the number density (for maximum deposition rate) and energy distributions (for desirable film microstructure) of all species present in the chamber. It is evident from the measurements of intrinsic chamber conditions that the behavior of the reactive sources is such that an optimization of this kind would be difficult to achieve using an "intuitive" approach, in which one makes educated guesses about optimum extrinsic processing conditions, and that plasma diagnostics facilitate intelligent process design.

O3.7
BIAS VOLTAGE INFLUENCE ON SURFACE MORPHOLOGY OF TITANIUM NITRIDE SYNTHESIZED BY DYNAMIC NITROGEN AND TITANIUM PLASMA ION IMPLANTATION AND DEPOSITION. Xiubo Tian, Langping Wang, Kingyu Fu, Paul K. Chu, Dept of Physics & Materials Science, City University of Hong Kong, HONG KONG.

Titanium nitride thin films are synthesized on AISI304 stainless steel substrate using dual titanium and nitrogen plasma in an immersion configuration. The titanium plasma is produced by a vacuum arc plasma source whereas the nitrogen plasma is sustained by hot filament glow discharge. A 30 microsec implantation duration and 270 microsec titanium arc duration are used to achieve both ion implantation and metal deposition. The impact of the implantation voltage on the film morphology is investigated using three voltages, 8kV, 16kV, and 23kV. Atomic force microscopy analysis reveals small islands on the surface of the 8kV sample. They are relatively smooth and more or less uniformly distributed on the surface. The surface morphology of the higher voltage samples is quite different. The density of the surface islands decreases but they bceome higher and steeper. On the 23kV sample, the hillocks become less uniform and appear like clusters of arrows. In addition to presenting the experimental results, we will discuss the mechanism by describing the impact of the implantation voltage on the growth dynamics of the coating and the relevant ion bombardment effects.

O3.8
$Ti_{1-x}W_xN$ FILMS WITH DIFFERENT TUNGSTEN CONTENTS. Ayako Kimura, Hiroyuki Hasegawa, Tetsuya Suzuki, Keio Univ, Dept of Mechanical Engineering, Yokohama, JAPAN.

Addition of second metals such as Al, Zr and Cr into TiN films substitutes some Ti atoms with these metals and provides higher hardness and improvement of wear resistant. For example, the crystal structure of (Ti,Al)N is kept cubic but the lattice parameter decreases in proportion to the Al content. For the practical purposes such as cutting tools and molds, there are many reports on (Ti,Al)N, (Ti,Zr)N and (Ti,Cr)N films based on hardness and wear resistance. On the other hand, few study has been reported on (Ti,W)N system because of experimental difficulties, although more attractive properties have been expected. In this study, we prepared $Ti_{1-x}W_xN$ ($0 < x < 1$) films using Ti and W targets by the arc ion plating method changing W contents. In this method, atoms or clusters, ejected from surface of targets, are ionized and reacted with process gases, and finally reach substrates as films. The Ti and W targets were simultaneously arc-discharged at an arc current of 0 - 100 A in order to change W content in $Ti_{1-x}W_xN$ films. The films were deposited on cemented carbide substrates which were biased at -20 V and at temperature of approximately 500°C under nitrogen plasma circumstance. After the film deposition, micro-hardness of films was measured by the conventional micro-Vickers hardness test comparing with the lattice parameters of the films. In this paper, we synthesize novel $Ti_{1-x}W_xN$ films films by changing the W ratio against Ti and measure their mechanical properties. Further, we discuss the potential use of $Ti_{1-x}W_xN$ films for practical purposes.

O3.9
A STUDY OF THE INTERACTIONS GUIDING THE FORMATION OF LAYER-BY-LAYER FILMS. Maria Raposo, Paulo António Ribeiro, Universidade Nova de Lisboa, Faculdade de Ciências e Tecnologia, Departamento de Física, Monte Caparica, PORTUGAL; Nara C. Souza, Osvaldo N. Oliveira Jr., Universidade de São Paulo, Instituto de Física de São Carlos, São Carlos, SP, BRAZIL.

The formation of layer-by-layer films is mainly based on electrostatic interactions since they are the result of polyelectrolyte adsorption from solution onto electrically charged surfaces. However, depending on the particular polyelectrolyte structure, interactions as hydrogen bonding can also play an important role in the film formation and consequently in the properties of a final device. In order to investigate the interactions responsible for the film cohesion a thermally stimulated desorption technique in solution was employed. In this technique, the temperature of the film solvent system is increased at a constant rate and the amount of desorbed material measured as a function of the temperature. Desorbed amount rate versus temperature curves reveal peaks from which activation desorption energies can be determined. Activation desorption energies of 75 kJ/mol and 220 kJ/mol were obtained in layer-by-layer films of poly(o-methoxyaniline) (POMA) alternated with poly(vinylsulfonic acid) (PVS). These values were attributed to hydrogen bonding and ionic forces, respectively. The presence of hydrogen bonding is the explanation for the adsorbed amount to be dependent on the concentration, in opposition to what one can expect from the adsorption of electrically charged polymers. Indeed, the adsorption of a layer onto a layer-by-layer film should be dependent on the number of electrical charges of the last adsorbed layer and, as a consequence, independent of the polyelectrolyte concentration.

O3.10
EVOLUTION OF INTERFACE DURING TOP FILM DEPOSITION: DIFFERENCE IN SURFACE ENERGIES. Victor Sapozhnikov, Recording Head Operations, Seagate Technologies, Minneapolis, MN.

A Monte Carlo simulation has been used to study how the difference in surface energies of the deposited films affects the stack structure. The simulation indicates that in a stack, segregation can considerably change the interface geometry and even the structure of the bulk. More specifically, it has been shown that: 1. Deposition of a film with higher surface energy upon a film with lower surface energy can lead to significant roughening of the interface. Thus, in stacks, interface morphology can be very different depending on the deposition order. 2. The atoms of the bottom film having low surface energy tend to float up and the atoms of the top film tend to dig into the first film. The two fluxes are not equal. The flux up is stronger than the flux down (the boundary conditions create asymmetry in the system). As a result of the differences in fluxes, vacancies, pores and pinholes form in the bottom film (the Kirkendall/Frenkel effect). This also makes the interface asymmetric. 3. In the lateral direction, similar processes take place. Once the diffusion flux of the top film atoms has reached the terrace edges, the bottom film atoms try to replace them and be at the edge. As a result, the terrace edges get rougher, similarly to the surface roughening. 4. Because surface diffusion is much faster than volume diffusion, segregation at the growing surface should be much easier than in the bulk. Therefore, the described phenomena take place until the second film has covered the first film completely. 5. Negative mixing energy (the components do not want to mix) suppresses the interface roughening. 6. The predictions of the model are in agreement with the experimental evidence on the effect of difference in surface energies on film growth.

O3.11
Abstract Withdrawn.

O3.12
REDUCED ORDER REPRESENTATIONS OF EPITAXIAL THIN FILM GROWTH. Martha A. Gallivan, David G. Goodwin, and Richard M. Murray, Division of Engineering and Applied Science, California Institute of Technology, Pasadena, CA.

Control of epitaxial thin film deposition processes requires a model that can predict, at least approximately, the change in film properties of interest resulting from changes in process conditions. For epitaxial films, kinetic Monte Carlo models are often used to simulate the evolution of surface morphology, but KMC models are usually too slow to run in real time, as required for control applications. Furthermore, most control strategies require that the system be described by a set of ordinary differential equations. We are investigating methods to take a specified KMC model and generate approximate ODE models that are able to reproduce the dynamic response of measurable outputs (e.g. roughness, RHEED signal) to changes in process conditions predicted by KMC. We begin by casting the KMC model into master equation form, which converts it into a linear system of ODEs, albeit with very high dimension (one ODE for each possible surface configuration). Standard techniques to reduce the dimensionality of large systems of linear ODEs are available, and here we explore their use to generate highly reduced ODE models that capture the important outputs of a KMC model. For a model problem, we find that the evolution of roughness as predicted by KMC is well-described by a system of 12 ODEs, which is easily small enough to use for real-time process control.

O3.13
THE INFLUENCE OF THE INTERNAL MICROSTRUCTURE ON THE SURFACE PARAMETERS OF POLYCRYSTALLINE THIN FILMS. C. Eisenmenger-Sittner, A. Bergauer Institut für Angewandte und Technische Physik, Technische Universität Wien, Vienna, AUSTRIA.

Physical Vapor Deposition (PVD) processes commonly lead to the formation of polycrystalline thin films due to the effects of island nucleation and growth. Scanning probe Methods such as Atomic Force Microscopy (AFM) or Scanning Tunneling Microscopy (STM) are widely used for the characterization of the film surface. The topographic data obtained from these measurements can be converted to roughness values, Power Spectral Densities (PSD's) or correlation functions. It is the objective of this paper to evaluate the possibilities to characterize the polycrystalline template which generates the film surface solely by quantities derived from topographic data. For this purpose roughness values, PSD's and correlation functions of polycrystalline Al-Films deposited on glass substrates and from simulated surfaces are compared. The main factors which influence the shape of PSD's and correlation functions are determined and

possible connections between the constitution of the polycrystalline template (e.g. shape and size-distribution of the crystalline domains) and the film roughness are discussed.

O3.14
ANGULAR DEPENDENCE OF THE DYNAMICAL SCALING BEHAVIOR IN LOW-MOBILITY MODELS OF THIN-FILM GROWTH. Jianguo Yu, Jacques G. Amar, Univ of Toledo, Dept of Physics & Astronomy, Toledo, OH.

We have studied the dynamical scaling behavior as a function of the sputter-angle distribution in two- and three-dimensional models of ballistic deposition with shadowing. In particular, we have studied two different distributions, a uniform angular distribution corresponding to high Ar pressure, and a "cosine" distribution corresponding to low or moderate Ar pressure. While in all cases, the resulting films are compact, in two-dimensions we find that there exist two distinct universality classes described by different values of the coarsening and roughening exponents p and β describing the evolution of the lateral feature size and surface roughness with film thickness, as well as of the surface fractal dimension D_f. In order to accurately determine the surface fractal dimension a novel dynamical scaling form was used. For the case of a uniform distribution we find $p = \beta = 1$ and $D_f \simeq 1.7$ while for a cosine distribution we find $p \simeq 2/3$ and $D_f \simeq 1.5$ while the roughening exponent β depends on microscopic details. In contrast, an angular distribution corresponding to a narrow range of angles with respect to the substrate normal leads to a self-affine surface. We conjecture that the scaling behavior is independent of the exact form of the angular distribution but depends primarily on the large-angle behavior. This is confirmed by results obtained for other angular distributions. The effects of surface diffusion on shadowing and on crossovers in the scaling behavior will also be discussed. Results for the case of three-dimensional ballistic deposition with both a cosine and uniform distribution will also be presented.

O3.15
NANOTRIBOLOGY STUDIES OF Cu/Cr AND TiB_2/Cu/Cr MULTILAYER THIN FILMS USING NANOINDENTATION AND NANOSCRATCH TECHNIQUES. G. Wei, J. Du, A. Rar and J.A. Barnard, Department of Metallurgical and Materials Engineering and Center for Materials for Information Technology, The University of Alabama, Tuscaloosa, AL.

The nanotribological behavior of dc magnetron sputtered Cu, Cu/Cr, TiB_2/Cu and TiB_2/Cu/Cr deposited on Si(100) has been studied using nanoindentation and nanoscratch techniques. The nanohardness and modulus of the thin films were measured by a Hysitron nanomechnical testing system. Constant and ramped load scratches were made using a Nano Indenter II system at various loads (30μN, 100μN and 1000μN). XRAY and XRAY reflectivity were used to measure the film structure and film thickness, respectively. Atomic force microscopy was used to evaluate the surface morphology and the scratch wear tracks of the films. The grain size and orientation of the Cu thin films were measured by TEM. To analyze the influence of Cr underlayer on Cu and TiB_2/Cu thin films, the hardness of Si(100) substrate and Cr thin flims were both measured. Although the hardness of Si (about 11$\sim$13GPa) is higher than Cr (about 8$\sim$10GPa), the hardness of Cu/Si and TiB_2/Cu/Si is lower than Cu/Cr/Si and TiB_2/Cu/Cr/Si respectively, indicating that the 2nm thick Cr underlayer may change the growth of the Cu thin films deposited on it. AFM images show that the roughness of Cu/Si thin films (RMS$\approx$3.1nm) is higher than Cu/Cr/Si (RMS$\approx$1.7nm). XRY diffraction patterns also indicate that the structure of Cu has been changed when deposited on the Cr underlayer. In the nanoscratch tests, the Cu and TiB_2thin films with Cr underlayers present higher critical load than the ones without Cr underlayers. For each of the four films, under the same load, the displacement in constant load scratch is higher than in the ramped load scratch. The mechanism responsible for this difference in displacement has been analyzed.

O3.16
LEVEL SET SIMULATION OF 3-D POLYCRYSTALLINE FACETED FILMS. Xingquan Li, Dept. of Physics, University of Michigan, Ann Arbor, MI; Peter S. Smereka, Dept. of Mathematics, University of Michigan, Ann Arbor, MI; David J. Srolovitz, Princeton Materials Institute, Princeton University, Princeton, NJ; Giovanni Russo, Dept. of Mathematics, University of L'aquila, ITALY.

We have developed a general purpose algorithm for the growth of polycrystalline, faceted thin films from the vapor based upon the level set method. The variation of the film microstructure and morphology with growth conditions (i.e., the relative growth rates of different crystalline facets) will be examined. The evolution of grain size, texture and surface roughness with film thickness will be presented. We will also present our simulation results on the growth of polycrystalline MgO film in the presence of a low energy ion beam, which is used to establish in-plane texture. We examine the development of the film microstructure and in-plane texture as a function of ion beam properties.

O3.17
STUDY OF ATOMIC STEPS ON THE SINGLE CRYSTAL SURFACE BY GRAZING ION SCATTERING. Abdurauf Dzhurakhalov, Institute of Electronics, Tashkent, UZBEKISTAN.

Ion bombardment of a solid surface leads to radiation-induced vacancy defects, atomic steps and their clusters, as well as the atomic scale relief formation. The concentration and the type of the radiation defects being formed depends upon the experimental conditions and significantly influences the trajectories, angular and energy distributions, as well as the number of the scattered particles. In the present study the low-energy Ne and Ar ion scattering from atomic steps on Cu(100) and GaP(100) surface at grazing incidence, their dechanneling effects have been investigated by computer simulation. The trajectories of the particles scattered both by the ordered part of the surface and the monoatomic steps of the different spatial extension placed upon it have been carefully studied in the binary collision approximation using the universal Biersack-Ziegler-Littmark interaction potential. Elastic and inelastic energy losses have been summed along the particle paths. Energy distributions of particles scattered by the isolated monoatomic steps (fragments) consisting of several atoms (from one to four) have been calculated. The distances between the steps vary from two lattice constants to 50$\AA$. The characteristic peaks in the energy distributions were explained by the features of trajectories of scattered particles. Comparison of calculated and experimentally measured energy spectra shown that the most likely ones turned out to be steps (fragments) consisting of two and three atoms separated by the parts of the ordered surface of the length 15-45$\AA$. It has been shown that, from the correlation of the experimental and calculated energy distributions of the scattered particles, one may determine a spatial extension of the isolated atomic steps and distance between them on the single crystal surface damaged by the ion bombardment. The dechanneling of ions from the monoatomic semi-infinite steps on the GaP(100) surface as well as the trajectories of these particles have been carefully studied. The energy and angular distributions of the dechanneling ions have been calculated. It was shown that the dechanneling ions form the characteristic peaks in the angular and energy distributions of scattered ions. The dechanneling mechanisms of particles moving under surface atomic steps are discussed.

O3.18
DEPOSITION OF Ru THIN FILMS PREPARED BY MOCVD USING DIRECT LIQUID INJECTION SYSTEM. Sang Yeol Kang, Cheol Seong Hwang, Hyeong Joon Kim, Seoul National University, School of MS&E, Seoul, KOREA.

The requirements for the chemical vapor deposition (CVD) of metal electrodes for the (Ba,Sr)TiO_3 (BST) capacitor of dynamic random access memory (DRAM) devices becomes more critical as the storage node height increases. With the three dimensional geometry of the capacitor, the plate electrode need to be deposited by CVD as otherwise the device may suffer from a reliability problem due to electrical leakage or chemical reactions. One candidate as a electrode material is Ru. This is due to its good electrical performance as an electrode, such as ensuring the low leakage current and large dielectric constant of the BST as well as Ta_2O_5 dielectric films, and the good etching property compared to Pt. In this research, high-quality Ru thin films with good electrical resistivities, as low as 15$\mu\Omega$·cm, were deposited at 325°Cby low-pressure Metalorganic CVD (LP-MOCVD) with a new precursor of $Ru(C_5H_4C_2H_5)_2$ [Ru(EtCp)$_2$]using Direct Liquid Injection system. Also we studied the effects of tetrahydrofuran which is the solvent of the precursor, on the deposition of Ru thin films.

O3.19
SURFACE INDUCED CHEMICAL ORDERING OF (001) FePd EPITAXIAL LAYERS GROWN BY MOLECULAR BEAM EPITAXY. D. Halley, Y. Samson, A. Marty, C. Beigne, CEA/DRFMC, Grenoble, FRANCE; B. Gilles, CNRS/LTPCM, Grenoble, FRANCE.

We investigated the ordering of equiatomic FePd epitaxial films deposited by MBE on Pd (001). This fcc alloy shows an ordered tetragonal CuAu (I) type structure (L10 phase) that attracts a considerable interest due to its magnetic anisotropy along the c-axis. Growths at room temperature yield disordered films, whereas growths at 620K yield well ordered alloys with the c-axis oriented in the growth direction, leading to alternated pure Fe and Pd (001) atomic planes parallel to the surface. By Scanning Tunnelling Microscopy on the surface of ordered films we observed mono and bi-atomic steps. As Electron Auger Spectroscopy showed that the upper plane at surface was pure Pd, due to segregation, we evidenced that bi-atomic steps

reflect the ordered structure of Fe-Pd bilayers, whereas monoatomic steps might be the emergence of antiphase boundaries within the L10 phase. This is confirmed by the oscillations of RHEED specular intensity during growth: the period corresponds to one atomic monolayer in the case of disordered films, and to two atomic layers in the case of ordered films. Moreover, disordered films grown at room temperature and next annealed for hours at 650K ordered with the c-axis along the three < 100 > directions, contrary to films grown at 620K. It suggests that the uniaxial ordering during growth is driven by surface processes, outlined by the formation of bi-atomic steps, the segregation of Pd selecting the c-axis perpendicular to the surface. Growths at intermediate temperature, between RT and 620K lead to partial ordering with the same c-axis. Observation of these samples by TEM and X-Ray evidenced a pseudo-periodic arrangement of anti-phased domains having a columnar shape whose size might be set by the diffusion length on the surface during growth.

O3.20
CHEMICAL ORDERING AND MICROSTRUCTURAL DEVELOPMENT IN NICKEL ALUMINIDE THIN FILMS. Gregory B. Thompson, Rajarshi Banerjee, Peter M. Anderson, Hamish L. Fraser, Dept of MS&E, Ohio State University, Columbus, OH.

Thin films of alloys and intermetallic compounds are finding increasing applications as structural coatings in the aerospace, microelectronics and magnetic recording industries. An interesting candidate for such coatings is the chemically ordered intermetallic compound Ni_3Al which has been extensively researched in the bulk form. This paper describes a novel study of the microstructural development in sputter-deposited polycrystalline thin films of Ni-25Al as a function of the substrate deposition temperature. Films were deposited on oxidized Si substrates at ambient temperature, 473K, and 673K. These films have been characterized by x-ray diffraction and transmission electron microscopy. The film deposited at ambient temperature exhibited a strong {111} fiber texture and a columnar grain morphology. However, in contrast to the behavior of sputter-deposited elemental metals, the films deposited above ambient temperatures consisted of refined microstructures and exhibited a low degree of texturing. This anomalous behavior has been explained by the role of exothermic heating accompanying chemical ordering and consequent formation of the $L1_2$ Ni_3Al phase in the films.

O3.21
EPITAXIAL GROWTH AND INTERFACE ROUGHNESS OF PdMn/Fe BILAYER STRUCTURES GROWN BY ION-BEAM SPUTTERING. Ning Cheng, Materials Science and Engineering Department, University of California Berkeley; Werner Grogger, J.P. Ahn and Kannan Krishnan, Materials Sciences Division, Lawrence Berkeley National Laboratory, University of California, Berkeley, CA.

Epitaxial PdMn/Fe/MgO bilayer structures were grown by IBS (ion beam sputtering) at different substrate temperatures. Different orientations of PdMn films and different stacking orders of PdMn and Fe on MgO(001) were studied. The interface roughness of these samples was characterized by energy-filtered transmission electron microscopy (EFTEM). The orientation relationships were confirmed by x-ray diffraction and TEM. The final PdMn orientation was determined by the competition between the growth kinetics and thermodynamic forces. At low temperatures (T< 280°C) dominated by the kinetics of growth, a-axis orientated [PdMn(100)/Fe(001)/MgO(001)] was stabilized whilst c-axis [PdMn(001)/Fe(001)/MgO(001)] were obtained at higher temperatures (T> 300°C) when the thermodynamics forces dominate. Spontaneous chemical ordering was found to occur in the c-axis films. As grown a-axis oriented films were disordered but after annealing (40 min, 230°C) showed evidence for substantial chemical ordering. In addition to the normal structure, inverted structures, Fe(001)/PdMn(001)/MgO(001) and Fe(001)/PdMn(100)/MgO(001), were obtained epitaxially for the first time. This growth was accomplished without the use of any seed layers. EFTEM images of cross-section samples have been analyzed using our recently developed quantitative interface-roughness extraction method. The interface roughness varies as orientation and growth sequence changes. A discussion of the roughness with growth conditions will be included. The magnetic exchange coupling (He) of these PdMn/Fe bilayers show a wide range in values: ~10 Oe for annealed a-axis samples, ~33 Oe for c-axis normal samples and ~68 Oe for c-axis inverted samples. (68 Oe is the biggest He so far published in this system) Further investigations are in progress to correlate He with the structure of the interface (roughness, spins).

O3.22
RELATION BETWEEN TEXTURE AND STRESS IN THIN MOLYBDENUM LAYERS. Ilse M. van den Berk, Léon J. Seijbel, Rob Delhez, Laboratory for Materials Science, Delft University of Technology, Delft, NETHERLANDS.

Pure Mo layers were deposited by magnetron sputtering at room temperature on an oxidized silicon wafer (100) at four sputter pressures: 0.25 Pa, 0.5 Pa, 1.0 Pa and 2.0 Pa respectively. The thickness of the deposited layers is 500 nm, the deposition rate was 16.7 nm/min at a power of 510 W (DC). X-ray diffraction was used to evaluate the stress and texture of the layers. All specimens show an almost perfect (110) fibre texture. A more or less appreciable part of the crystals also show a preferred in-plane orientation with (110) planes perpendicular to the rotation direction of the sputter table. The $\sin^2\psi$-method was used to determine the stress in the layers. By measuring the strains for two specimen orientations, i.c. the crystal orientations corresponding to the minima and maxima of the in-plane texture, the stresses could be determined for the predominant orientations of the in-plane texture and for the orientations corresponding to only the fibre texture. The stress states observed are tensile and not rotationally symmetric. Heat treatments at 600 and 800 K were performed on the layer deposited at 0.5 Pa. It was found that no change occurred in the texture. The absolute magnitude of the stress in the layer decreased indicating a decrease of the intrinsic or growth stress. At the same time the (direction independent) thermal stress increased and the stress state became more rotationally symmetric. This paper explains the differences in stress and texture in relation to the sputter pressure.

O3.23
MICROSTRUCTURE AND ELECTRICAL PROPERTIES OF INTERMEDIATE RARE-EARTH METAL LAYERS FOR MEDIUM-K DIELECTRIC APPLICATIONS. Nabil D. Bassim, V. Craciun, J. Howard, R.K. Singh, Department of Materials Science & Engineering, University of Florida, Gainesville, FL.

The development of high-K dielectric materials to replace SiO_2 as the gate oxide in silicon-based MOS device structures has attracted much interest recently. One of the key challenges in producing oxide thin films has been to prevent the formation of an interfacial layer of SiO_2 between the film and the substrate, which subsequently reduces the effective gate oxide capacitance. One possible solution to this problem is the deposition of an intermediate metal layer that is more stable with the substrate than SiO_2. and which, when annealed in an oxygen ambient, can form a thermodynamically stable very thin rare-earth silicate or oxide layer upon which a medium or high-K capping layer can be deposited. Thin (~15 A) zirconium and hafnium layers were deposited using pulsed laser deposition techniques and annealed in an oxygen atmosphere to form a stable silicate layer and ZrO_2 and HfO_2 films were subsequently deposited in order to raise the K value of the structure. Cross-sectional high-resolution transmission electron microscopy and X-ray photoelectron spectroscopy were used to investigate the layers formed in this composite structure and the microstructure and processing parameters were related to the measured Capacitance-Voltage and Current-Voltage characteristics of the film.

O3.24
TEXTURE IN THIN FILMS: Nb/Al, Ti/Al AND Al. Wayne Archibald, Katayun Barmak, Carnegie Mellon University, Dept. of Materials Science and Engineering, Pittsburgh, PA; Gene Lucadamo, Lehigh University, Dept of Materials Science and Engineering, Bethlehem, PA.

Texture in Ti/Al and Nb/Al polycrystalline multilayer thin films, with bilayer thicknesses ranging from 20 to 333 nm and having a fixed stoichiometry of 1/3, and pure Al films with thicknesses ranging from 0.25 to 1 micron, has been investigated using x-ray pole figures and transmission electron microscopy. Two sets of multilayer films were deposited; one set contained pure Al and the other Al-1.0 weight percent Cu. The texture was found to be strengthened by the formation of a coherent superlattice for the Nb/pure Al film with the smallest bilayer thickness. By contrast, the texture in Ti/pure Al films with a similar period was not as strong. The strength of texture also decreased with increasing bilayer thickness for both the Ti/pure Al and Nb/pure Al films. Near < 111 > fiber texture, rather than < 111 > fiber texture, was observed for both sets of films prepared with Al/1.0 weight percent Cu. Here, an increase in the width of the Al(111) peak and an offset of the fiber axis from the substrate normal by as much as 8 degrees was observed in films with thickness of 333 nm. The decrease in multilayer texture upon addition of Cu to Al was attributed primarily to an increase in interlayer roughness as a consequence of reduction in the Al(Cu) grain size. For single layer pure Al films, the strength of texture was found to increase with increasing thickness. Near < 111 > fiber texture was observed in all cases. The results of our investigations were interpreted in the context of structure zone and dynamic roughness models of film growth.

O3.25
MICROSTRUCTURE EVOLUTION OF ELECTROPLATING DEPOSITED NICKEL AS A FUNCTION OF PROCESSING PARAMETERS. Kun Lian, Center for Advanced Microstructures and

Devices, Louisiana State Univ, Baton Rouge, LA; Dean Guidry, Jie Chao Jiang, E.I. Meletis, Mechanical Engineering Dept, Louisiana State Univ, Baton Rouge, LA.

Electroplated Ni is the major material used currently in Microelectromechanical Systems. In the past, very little work has been done to study the relationship between Ni electroplating parameters and resulting microstructures. The present work is focused on the processing-structure-mechanical property relationship of electroplated Ni. A sulfamate bath was used to produce Ni electrodeposits. Electroplating temperature and current density were varied between 37°C-50°C and 5 mA/cm^2-30 mA/cm^2, respectively to produce 50 μm thick Ni layers with a grain size ranging from 70 nm to 100s nm. The structures of the layers produced at the various processing conditions were characterized by cross sectional TEM. Nanoindentation tests were conducted to assess hardness and elastic modulus of the Ni layers. Pin-on-disc experiments were performed to study the tribological behavior. The relationship between grain size and mechanical properties is discussed.

O3.26
CRYSTALLOGRAPHIC AND MORPHOLOGICAL PROPERTIES OF MAGNETRON SPUTTERED Ti AND Zr THIN FILMS. Eliane F. Chinaglia, Ivette C. Oppenheim, University of São Paulo, Institute of Physics, São Paulo, SP, BRAZIL.

The microstructure of polycrystalline hcp Ti and Zr thin films was analyzed with Atomic Force Microscopy and X-ray Diffraction. The films were deposited by magnetron sputtering on amorphous substrates (SiO_2 over Si). The used Ar gas partial pressure and the deposition rate were 0.8mTorr and 0.09nm/s, respectively. The surface morphology and crystallographic properties of the films were studied as a function of the homologous temperature ($0.15 \leq T_S/T_M \leq 0.43$, where T_S is the substrate temperature during deposition and T_M is the melting point of the film material) and film thickness (43nm$\leq$ t $\leq$278nm). At low temperatures (T_S/T_M=0.15), Ti and Zr films have an {0002} preferential texture. The texture and the crystalline grain size do not depend on the thickness of the films. As a consequence of low surface diffusion and grain boundary mobility, the surface morphology is composed by small grains and compact grain boundaries. The well-defined crystallographic texture suggests that the initial nucleation is formed by islands with preferential orientation. As T_S/T_M increases, the {0002} texture of the Zr films improves. The higher is the temperature, the thinner are the films that present a dominant {0002} preferential texture. For the Ti films, as T_S/T_M increases, the {0002} texture decreases giving rise to a $\{10\bar{1}1\}$ texture. At T_S/T_M=0.43, the Ti films present a dominant $\{10\bar{1}1\}$ texture. In general, increasing the deposition temperature leads to an increase in the average grain diameter, and as the film thickness increases, the texture improves and the crystalline grain size increases. The growth rate of the average grain diameter as a function of thickness is higher for the Ti films than it is for the Zr films. The evolution of surface morphology and texture of the films suggest that the Zr films present an almost columnar structure while the Ti films are formed by grains with a cone-like shape as a consequence of competitive grain growth.

O3.27
COMPARISON OF THE ATOMIC PEENING EFFECT IN SPUTTER-DEPOSITED EPITAXIAL AND POLYCRYSTALLINE Pd/Pt MULTILAYERS. V. Ramaswamy, W.D. Nix, and B.M. Clemens, Stanford University, Dept. of Materials Science and Engineering, Stanford, CA.

Energetic bombardment of films during sputter deposition by reflected neutral gas atoms (typically Argon) and target atoms, also known as *atomic peening*, has a pronounced effect on film stress and microstructure. The bombardment energy, and hence the degree of peening, decrease as sputtering gas pressure is increased, due to increased thermalization. Differences in stress generation due to atomic peening in polycrystalline and epitaxial layers are studied using *in situ* substrate curvature measurements during sputter deposition of Pd/Pt multilayers. Coherency stresses, based on bulk lattice mismatch, are compressive for Pt and tensile for Pd. Stress behavior of Pt layers in epitaxial and polycrystalline samples is similar; at low Argon pressures, large compressive stresses consistent with coherency and atomic peening develop in the Pt layers. At high Argon pressures, Pt layers are in tension after initial coherency-related compressive behavior. The behaviors of polycrystalline and epitaxial Pd layers, however, are markedly different. While some peening-related compressive stress is observed in polycrystalline Pd at low Argon pressures, it is absent from the epitaxial Pd layers. In fact, epitaxial Pd layers sustain high tensile stress, likely due to coherency, and are insensitive to changes in sputtering gas pressure. This difference in stress behaviors of epitaxial and polycrystalline Pd is attributed to differences in microstructure of the layers. Observed stress behaviors in Pt and Pd are discussed in terms of sample microstructure, and surface morphology. A simplified one-dimensional diffusion model for defect incorporation during thin film growth provides useful insight into the various deposition parameters and material properties related to the atomic peening effect.

O3.28
THE STAGES OF STRUCTURE-ENERGETICAL TRANSFORMATIONS AT COMBUSTION SYNTHESIS IN THE SYSTEMS NiAl AND TiAl. Michail D. Starostenkov, Gennadiy M. Poletayev, General Physics Dept, Altai State Technical Univ.

It is known, that combustion synthesis (CS) takes place at high velocities. That is why it is difficult to determine the stages of structure-energetical transformations, taking place at CS. The process of CS is modelled by the computer simulation, using molecular dynamics method. The investigating systems are presented in a form of bimetal thin films at the beginning of the process. The interactions between the atoms are given by the sets of emperic pair potentials. The set of critical parameters, regulating the velocity of the reaction of CS is found in the result of computer experiment. The parameters are the following: limited free volume, it's connection with the temperature of the process beginning, the velocity of components mixing, the velocity of formation of intermetallic phases. It is established, that the structure transformations of the system take place at the formation of nanocrystal phases in the process of CS.

O3.29
MICROSTRUCTURE ORIGIN FOR THERMAL FATIGUE OF TiNi FILMS. Shulin Wen, Shandong University, Dept of Material Science and Engineering, Shandong, CHINA.

Fatigue is a progressive and localized permanant structual change. It occurs in such a material which subject to repeated and fluctuating stain. Fatigue occurs in TiNi shape memory alloy (SMA) during its application due to repeated and fluctuating stains at low-high temperature cycling. One of the goals of TiNi SMA application is to make miniature valve as smart microvalve which is applied to combustion engine fuel delivery system or closed-loop con trol drug delivery system. The material used for this purpose needs to work for mollions of low-high temperature cycles at least. Fatigue then occurs and the decay of the performence of SMA first and then further fracture produced. Therfore , it is very important to investigate the micrstructural origin of this fatigue in order to retain the SMA performence as long as possible in life. The parent phase in present TiNi films has B2 structue, on cooling it may transfom martensitically to B19" and R phases. Present investigation results showed that a small amount of B2 phase did not transform to B19' and R phases due to dynamical resean and a little amount of H phase formed during this martensite transformation. Present investigation also indicated that there some precipitates produced in the fatigued specimens. The precipitates which are responsible for the fatigue were obvserved in the fatigued specimen as trace phase with grain size of 10-20 nm. it could be identified as $TiNI_3$ phase from our TEM image, electron diffraction pattern and EDS results. To effectively control these precipitates is the key to improve the SMA film performence life.

O3.30
MICROSTRUCTURE, STRESS AND MECHANICAL PROPERTIES OF ION BEAM SPUTTER DEPOSITED, METAL HYDRIDE THIN FILMS. David P. Adams, Neville R. Moody[a], Juan A. Romero, Jerry Floro, Ronald Goeke, and Mark Rodriguez, Sandia National Laboratories, Albuquerque, NM. [a]Livermore, CA.

We investigate the microstructure, stress and mechanical properties of reactively sputtered metal hydride thin films. Metal hydride films are currently of interest for miniature fuel cells, down-hole oil logging devices and switchable mirrors. In present work, the development of metal hydride film microstructure is studied as a function of the growth parameters. This includes analysis of crystal texture and phase for rare earth metal hydrogen compounds, including erbium hydride. Films are deposited onto several different substrates (Si(100) having native oxide, molybdenum, a-plane Al_2O_3 and c-plane Al_2O_3) in order to determine the influence of the starting surface. Thin film stress is monitored during each stage of fabrication including nucleation, growth and post-deposition cooldown using a laser based, multi-beam wafer curvature sensor. Stress developed during deposition is correlated with changes in morphology, microstructure and composition. Extrinsic stress is probed after deposition to accurately determine coefficients of thermal expansion. These results suggest that strain energy influences the stability of certain rare earth metal hydride crystal phases. Furthermore, we evaluate the mechanical properties of films using nanoindentation and nanoscratch techniques. These tests determine the elastic moduli and interfacial toughness of metal hydride films.
This work was performed at Sandia National Laboratories and is supported by the United States Department of Energy under contract no. DE-AC04-94AL85000. Sandia is a multiprogram laboratory

operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy.

O3.31
THE LASER-MOSSBAUER METHOD FOR SURFACE EVOLUTION AND THIN FILM MICROSTRUCTURE.
Monica Sorescu, Duquesne University, Physics Department, Pittsburgh, PA.

The laser-Mossbauer method is a method pioneered in our laboratory for the study of amorphous magnets and their nanostructures. It is a new method, of a hybrid type: processing-characterization. The method combines an extremely sharp tool for exciting the amorphous structure with a characterization technique that has the highest resolution known in Physics. We shall demonstrate that this method yields amorphous magnets with controlled properties. Using amorphous FeBSiC, FeNiMoB, FeCoBSi and FeCrAlSiY as model systems, we applied the laser-Mossbauer method in order to obtain metallic glasses with novel properties. As shown by transmission Mossbauer spectroscopy, the bulk magnetic texture was modified in a rational manner by applying a varying number of excimer laser pulses per spot. As shown by conversion electron Mossbauer spectroscopy (CEMS), this process left the surface magnetic texture unchanged and induced a distribution of magnetic moment directions through the thickness of the foil. A similar dependence of the magnetic texture on the number of applied laser pulses was obtained in metallic glasses irradiated with a Nd:YAG laser. However, in this case we observed the onset of surface crystallization using the hyperfine magnetic field distributions extracted from the CEMS spectra. When a pulsed alexandrite laser was used, the onset of crystallization was found to be accompanied by bulk oxidation and the formation of magnetite nanoparticles in the irradiated system. Finally, a crucial experiment was performed in order to demonstrate the role played by the magnetostriction constant in the onset of crystallization. Consequently, the laser-Mossbauer approach made it possible to obtain unique information on the surface evolution and thin film microstructure, as well as produce materials with new types of magnetic moment distributions, not obtainable by conventional methods.

O3.32
THE FABRICATION, THE STRUCTURAL AND SURFACE STUDIES OF RARE-EARTH HEXABORIDE THIN FILMS.
Zhenchen Zhong, Institute for Micromanufacturing (IfM) and Physics Program, Louisiana Tech University, Ruston, LA; and Department of Physics, Grambling State University, Grambling, LA.

Rare-earth hexaboride ReB6 (Re = Gd, Ce and Nd) thin films were fabricated by a novel laser-initiated chemical processing Laser-induced deposition form solution (LISD). The Structures and Surfaces were studied by scanning electron microscope (SEM), X-ray emission spectroscopy (XES), and X-ray diffraction (XRD). We found that these films grew with a strong texture axis. The microstructure and surface evolution in the deposited films are dependent both on the choice of solvents and laser parameters (e.g, wavelength, laser power etc) used in LISD. Rare-earth hexaborides are typically low work function materials. They can be applied as cathodes in DC plasma display panels and micro X-ray tubes.

O3.33
MOCVD ZnS:Mn FILMS: GRAIN SIZE DISTRIBUTION AND CRYSTAL STRUCTURE AS A FUNCTION OF THE GROWTH PARAMETERS.
K. Dovidenko, K. Dunn, A. Topol, L. Senapati, S. Oktyabrsky and A.E. Kaloyeros, NYS Center for Advanced Thin Film Technology, the University at Albany-SUNY, Albany, NY.

Zinc sulfide doped with manganese is a promising material for thin film electroluminescence device applications. In order to fully assess the key material and process challenges, the ZnS:Mn layers were fabricated by the metalorganic chemical vapor deposition on the AlTiO/InSnO/glass stack, and the growth kinetics and correlation between the crystal structure and the electroluminescence performance were studied. The ZnS:Mn films were grown in the 250-500C temperature range, and fully characterized by the variety of structural and chemical characterization techniques such as Rutherford Backscattering, Secondary Ion Mass Spectroscopy, X-ray Diffraction, Scanning Electron Microscopy, Atomic Force Microscopy and Transmission Electron Microscopy (TEM). For all the growth conditions, the films were found to be polycrystalline having predominantly 2H hexagonal ZnS structure. The presence of the 8H ZnS polytype was detected in the low-temperature ZnS:Mn films by the TEM selected area electron diffraction and XRD measurements. The ZnS grains are found to grow columnar as the film thickness increases, also widening in the direction parallel to the substrate surface and reaching the 100 - 200 nm average lateral size at the 700 nm film thickness. Two types of grains were found in the low-temperature ZnS layers: small-sized (average 2.5 nm) and large-sized (average about 50 nm as measured at the 200 nm film thickness). For the high-temperature films, no grains smaller than 40 nm were observed, the average being between 50 and 65 nm (measured at the film thickness of about 200 nm). The small-size grains in the low-temperature films were present all the way through the ZnS layer thickness with a little bit higher density at the ZnS/ATO interface. These small-size ZnS grains were attributed to the 8H hexagonal polytype. The correlation of the grain microstructure with the electroluminescence behavior is discussed.

O3.34
MORPHOLOGY EVOLUTION KINETICS OF HOMOEPITAXIAL STRONTIUM TITANATE FILMS.
J.Y. Lee, S.F. Chen, J.Y. Juang, J.Y. Lin, K.H. Wu, T.M. Uen, Y.S. Gou, National Chiao-Tung Univ, Dept of Electrophysics, Hsinchu, TAIWAN.

The kinetics of surface morphology evolution of pulsed laser deposited strontium titanate (STO) homoepitaxial films was investigated by in-situ monitoring the intensity variations of reflection high-energy electron diffraction (RHEED) over a continuous annealing scheme. It was found that, independent of the temperature rising rate, an abrupt increase of RHEED intensity accompanied by the appearance of sharp diffraction spots always occurs around 660°C, indicative of a noticeable reduction of surface step density induced by surface morphology evolution. The temperature derivative of the RHEED intensity curve displays a resonance-like peak around 660°C, suggesting that a Langivan-type force equation might be applicable in describing the kinetics. Analogies of the present observations to flux creep governed by individual pinnings are discussed.

O3.35
THE INFLUENCE OF PLASMA COMPOSITION AND APPLIED POWER ON THE PROPERTIES OF PLASMA TREATED BIOMATERIALS.
Nilson C. Cruz, Elidiane C. Rangel, Giovana Z. Gadioli, Rogério P. Mota, Roberto Y. Honda and Mauricio A. Algatti, UNESP - Campus Guaratinguetá, Dept of Physics and Chemistry, Laboratory of Plasmas and Aplications, Guaratinguetá, SP, BRAZIL.

The response of a biological environment when in contact with an artificial material is primarily determined by material surface properties. Owing to that, different treatments have been employed to improve the performance of biocompatible materials. In this sense, plasma based- techniques are of particular interest because they enable the surface processing of materials with virtually any geometry, preserving bulk properties. In this work, glow discharge plasmas and Plasma Immersion Ion Implantation (PIII) techniques have been applied in the treatment of metals (Ti and Ti6Al4V) and polymers (PTFE, ultrahigh molecular weight polyethylene and PMMA) largely employed in clinical and orthopedic devices. Plasmas of inert (He and Ar) and reactive (O_2, N_2 and SF_6) gases were generated in a vacuum chamber by applying radiofrequency power (13.56MHz, 0-300W) to two external electrodes. In the PIII experiments the samples were biased with high voltage (25kV, variable frequency) negative pulses. The treatments were performed in different conditions of plasma composition and applied power. Nanoindentation and pin-on-disc techniques were employed to evaluate hardness, friction coefficient, and scratch and wear resistances. An automated goniometer using the sessile drop method was employed to determine contact angle and surface energy while elemental and structural modifications were determined by x-ray photoelectron and infrared reflectance-absorbance spectroscopies. It has been observed that the properties of the treated samples are extremely sensitive to plasma parameters. For instance, the contact angle of PTFE varied from 150 to 60 degrees when the oxygen partial pressure in the plasma ranged from 5 to 200 mTorr.

O3.36
THE INFLUENCE OF PARTICLE FLUX DENSITY AND SUBSTRATE TEMPERATURE ON TEXTURE FORMATION IN TUNGSTEN CARBIDE ION-PLASMA CONDENSATES.
Liliya I. Gladkikh, Oleg V. Sobol', Elena A. Sobol', Anatoly A. Podtelezhnikov, Kharkov State Polytechnical University, Dept. of Physics of Metals and Semiconductors, Kharkov, UKRAINE.

The energy (E_a) required to overcome the kinetic barriers for the atomic motion on a metal surface and to provide the occupation of energetically favorable sites by adsorbed atoms and thus to form a low-energy surface configuration is defined by the relation $E_a \geq 3K_b T_m$ (T_m is the melting temperature), and is for different materials it is in the range 0.2 - 0.8 eV. Under ion-plasma sputtering, the energy of deposited particles is much more 1 eV. In this case, radiation factor contributes to free energy of formed surface. It is particularly important to take this into consideration for deposition of two-component materials, such as transition metal carbides. In this case, heavy metal atoms deposition is accompanied by bombardment with light carbon atoms. For tungsten carbide with fcc - lattice, this results in the fact, that at critical flux density of depositing particles $(1 - 1.2)10^{15}$ cm^{-2} s^{-1}, formation of [100] texture becomes

energetically preferable and provides the least damage ability of NaCl-type crystal lattice. In addition, light carbon atoms get the possibility channelin to grain boundaries that result in vacancy occurrence in carbon sublattice of tungsten carbide. Increasing temperature under condensation up to 450 - 500°C results in decreasing critical particle flux density to 7 10^{14} cm^{-2} s^{-1}. At deposition temperatures higher 650°C, intensive carbon desorbtion from the surface changes substantially elemental composition of growing coating. It was found that vacancy presence in carbon sublattice causes decreased ratio of elastic modules $E_{(100)}$ / $E_{(111)}$. Such variation is probably characteristic for all transition metal carbides, but especially it reveales itself in carbides with strong binding Me-Me (TaC, MoC, WC). For explanation of experimental effects, calculation models are proposed.

SESSION O4: MULTILAYERS: STRESS IN THIN FILMS
Chairs: Roy Clarke and Jeffrey M. Rickman
Wednesday Morning, April 18, 2001
Salon 7 (Marriott)

8:30 AM *O4.1
ATOMIC SCALE STRUCTURE OF GIANT MAGNETORESISTIVE MULTILAYERS. H.N.G. Wadley, X.W. Zhou, R.A. Johnson, Dept of MS&E, University of Virginia, Charlottesville, VA.

The emergence of metal multilayers that exhibit giant magneoresistance has led to new magnetic field sensors, and new approaches for making nonvolatile random access memories. Controlling the atomic scale structure across the interfaces of these multilayers significantly improves the properties of these devices. However the ability to manipulate atomic arrangements at this scale requires an understanding of the mechanisms that control hetero metal film growth during vapor deposition. It is important to both measure the position and identity of atoms at the atomic length scale, and develop theoretical methods to assess the effects of deposition conditions upon this structure. Atomistic simulation approaches have been developed to achieve this, and have been applied to analyze the atomic scale structure of sputter deposited CoFe/Cu/CoFe giant magnetoresistive multilayers used for magnetic field sensing. Significant intermixing is revealed at the CoFe on Cu interface, but not at the Cu on CoFe interface. The use of processing conditions that inhibit thermally activated atomic diffusion coupled with impact energy control of the metal atom flux provides an effective means for control of the structure. A novel deposition process for the acheivement of this control has been designed and found to produce superior films.

9:00 AM O4.2
EPITAXIAL NiO-Co EXCHANGE-BIASED BILAYERS GROWN ON MgO SINGLE CRYSTALS: INFLUENCE OF THE SUBSTRATE ORIENTATION ON THE FILM MORPHOLOGY AND THE MAGNETIC BEHAVIOR. E. Snoeck, B. Warot, J.C. Ousset and M.J. Casanove, CEMES-CNRS,Toulouse, FRANCE; S. Dubourg, A.R. Fert and J.F. Bobo, LPMC-CNRS INSA, Toulouse, FRANCE.

We have sputtered Co/NiO bilayers on MgO (001) and (110) substrates. Epitaxial growth of NiO/MgO was evidenced by RHEED, X-ray diffraction and HRTEM experiments. Flat NiO (001) surfaces were obtained on MgO (001) with square-on-square epitaxy. The Co grows in its fcc structure when deposited on NiO(001) at room temperature with the relative orientation Co(001)[100]//NiO(001)[100]. This microstructure yields a four-fold in-plane anisotropy with the Co magnetic easy axes aligned along the NiO [110] directions. When the bilayer is annealed up to 300°C, the anisotropy axes switch to the [100] and [010] directions, the Co remaining fcc. In contrast, the Co layers deposited at 300°C and field-cooled to room temperature exhibit a hcp crystal structure with the c-axis aligned in the plane along either the NiO [100] or [010] direction. This induces the appearance of two Co domains having their c-axis perpendicular. The resulting magnetic easy axes are aligned along the NiO [110] directions. For NiO deposited on MgO (110), we observe a self-organized roof-structure growth by HRTEM, RHEED and AFM. To minimize its surface energy, the NiO (110) grows with (001) and (010) facets whose width varies with the deposition temperature from 7 to 14 nm. These facets are elongated along the [001] NiO direction and can reach several micrometers long. The Co layers grow in the fcc structure conformably on these facets. Such a morphology induces both a strong in-plane uniaxial anisotropy along [001] and an exchange bias along the same direction. Our results emphasize the role played by the crystal structure and the morphology of the layers on exchange bias.

9:15 AM O4.3
THE EFFECT OF SURFACTANTS ON THE GROWTH OF SPUTTERED Co/Cu MULTILAYERS. Brennan L. Peterson, Bruce M. Clemens, Robert L. White, Stanford University, Department of MS&E, Stanford, CA.

In the growth of metal films on metal substrates, surface structure and kinetics play a very important role. By modifying the growing surface with an additional material (a surfactant), the growth mode and resultant film properties can be altered. In magnetic films, the final properties are particularly sensitive to the film morphology and growth process. Cobalt/copper multilayers thus present an useful and relevant test case for surfactant assisted growth, with good lattice matching, but very different surface energies and diffusivities. X-ray, *in-situ* STM, and *in-situ* stress measurements were carried out on a series of [Co/Cu] films, using Pb and In as surfactants. DC magnetron sputtered [Co/Cu] multilayers were deposited on SiO_2 and chemically etched Si substrates. The *in-situ* stress was measured to determine surface energy effects. Stress was roughly consistent with epitaxial mismatch strains, and total film stress is significant. $\theta/2\theta$ and non-specular x-ray measurements were taken to determine the roughness scaling in the multilayer. Surfactant assisted growth showed a modestly decreased roughness (from 6 Å to 5 Å), and increased lateral scaling length. The effect appears to be mainly confined to the interface between Co and the Cu underlayer. Various models of surface growth and roughness scaling were also investigated, and the resultant fits compared. The choice of a scaling law has significant influence on fitting the data, especially in these relatively rough films. The films were then investigated on a chamber equipped with a DC magnetron sputtering chamber equipped with *in-situ* STM capabilities. X-ray determined scaling lengths and those determined from surface power spectra are related to grain size, island spacing, and ledges.

9:30 AM *O4.4
GROWTH AND STRUCTURE OF ULTRA-THIN X-RAY MULTILAYER STRUCTURES PREPARED BY MAGNETRON SPUTTERING. David L. Windt, Columbia University, Columbia Astrophysics Laboratory, New York, NY.

I will describe research directed at the development of multilayer structures prepared by magnetron sputtering, to be used as X-ray reflective coatings for X-ray astronomy. These thin film structures require maximally smooth and sharp interfaces between polycrystalline and/or amorphous layers of optically dissimilar metals, alloys, insulators and semiconductors. Typical structures may contain as many as 1000 layers or more, with individual layer thicknesses ranging from less than 1 nm to several tens of nm. The achievable level of interface perfection is crucial for optimal performance: interface imperfections (i.e., interfacial roughness and/or diffuseness) typically must be less than 0.3 nm. I will present recent results from both experiments and atomistic computer simulations of thin film growth that illustrate the critical role of a variety of sputter deposition conditions (e.g., background pressure, source collimation, sputter gas pressure, etc.) on film microstructure, interface morphology and stress, and demonstrate how such deposition parameters can be controlled in order to maximize performance.

10:30 AM *O4.5
MODEL FOR INTRINSIC STRESS DURING THE EARLY STAGE OF POLYCRYSTALLINE FILM GROWTH. R.C. Cammarata, T.M. Trimble, Johns Hopkins Univ., Dept. of Materials Science and Engineering, Baltimore, MD; D.J. Srolovitz, Princeton Univ., Princeton Materials Institute, Princeton, NJ.

A simple model for intrinsic stress generation in polycrystalline films resulting from effects of surface stress will be presented. This mechanism can explain the development of compressive intrinsic stresses often observed during the early stage of island growth. A physical picture for the generation of this stress is based on two effects. First, surface stresses acting on an unconstrained island induce an equilibrium lattice spacing different from that of the bulk solid. Second, there a critical size where the island first becomes firmly anchored to the substrate. As a result of this latter effect, an island larger than the critical size is no longer able to change its in-plane lattice spacing during further growth. Since the equilibrium lattice spacing will change as the island increases in size, the substrate must impose a traction to keep the island from attaining the equilibrium spacing. If a post-critical island has a smaller in-plane lattice spacing relative to bulk, corresponding to a positive surface stress, this traction will result in a compressive intrinsic stress. A simple, linear elastic analysis of the mechanism incorporating the thermodynamics of surface stress will be presented. It will also be discussed how this mechanism may contribute to a sudden change in the intrinsic stress during island coalescence as well as explain compressive intrinsic stresses observed in certain fully grown polycrystalline films.

11:00 AM O4.6
THE DYNAMIC COMPETITION BETWEEN STRESS GENERATION AND RELAXATION MECHANISMS DURING VOLMER-WEBER FILM GROWTH. J.A. Floro and S.J. Hearne,

Sandia National Laboratories, Albuquerque, NM.

We will show that a complex evolution of film stress from compressive to tensile to compressive (CTC) occurs during the initial stages of Volmer-Weber thin film growth. This generic behavior is observed over a wide range of crystal structures, including amorphous, and over a wide range of homologous deposition temperatures. This talk will focus on stress evolution in amorphous Ge films grown on silicon oxide in ultra-high vacuum. Using isothermal anneals, it is shown that intrinsic CTC behavior is still observed at room temperature, even though relaxation is fully suppressed. At higher temperatures, where relaxation does occur, discontinuous amorphous-Ge films initially in tension are observed to relax into net compression. This behavior is consistent with stress relaxation mediated by surface diffusion. Furthermore, this result, combined with stress evolution results from polycrystalline Ge, suggests that tensile and compressive stress generation mechanisms are operating simultaneously during island growth and coalescence. We will also show, by comparing stress evolution in Ag and Al films deposited on silicon oxide, that interfacial shear occurs efficiently in Ag islands, whereas this mechanism is suppressed in the more strongly-bound Al islands. In all the films studied here, relaxation ceases when the films become fully continuous. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

11:15 AM O4.7
EXPERIMENTAL INVESTIGATIONS AND FINITE ELEMENT MODELING OF INTRINSIC STRESS EVOLUTION DURING POLYCRYSTALLINE FILM GROWTH. A. Rajamani, A. Lau, J.R. Beresford, E. Chason and B.W. Sheldon, Brown University, Department of Engineering, Providence, RI.

Island coalescence during Volmer-Weber growth can produce large tensile stresses in polycrystalline films, particularly in systems where atomic mobilities are relatively slow. Recent models describe these stresses in terms of an energetic tradeoff between elastic strain and surface/interface energies, where the stress is generated only when initial island coalescence occurs. This is not consistent with the experimental results that we have obtained in several different systems (e.g., MBE nitrides and CVD diamond). In particular, the stress evolution appears to be more closely linked to the film growth kinetics, and this is not incorporated into these other models. We will present a new finite element model that accounts for stress generation during island coalescence and growth. This model is correlated with our experimental results, and also considers some of the likely stress relaxation effects (e.g., grain boundary diffusion). These coupled experimental and modeling efforts make it possible to predict the dependence of film stress and stress distribution on the film growth conditions.

11:30 AM O4.8
CHARACTERIZATION OF FILM GROWTH MODES BY *IN SITU* SUBSTRATE CURVATURE MEASUREMENT. V. Ramaswamy, W.D. Nix, and B.M. Clemens, Stanford University, Dept. of Materials Science and Engineering, Stanford, CA.

In situ substrate curvature measurements are used to study the mode of growth of sputtered Ag and Au films on (111)-oriented, polycrystalline and epitaxial Pd and Pt seed layers. Curvature measurements indicate that in both polycrystalline and epitaxial samples, the first 2 monolayers of Ag grow pseudomorphically and, subsequently deposited Ag is fully relaxed. In-plane lattice parameter measurements verify these results. Surface morphology characterization shows that coherently strained Ag layers wet the Pd and Pt underlayers, improving surface quality, while relaxed Ag roughens. Similar 2-D to 3-D transitions have been seen during MBE growth of Ag on single crystal Pt substrates, and are believed to be due to the larger step-edge barrier of relaxed Ag compared to compressively strained Ag[1] . It is remarkable that the growth behavior of Ag is insensitive to significant variations in the deposition rates and energetics between MBE and sputter deposition, and in the quality and structure of the growth surface. The stress evolution during deposition of Au on epitaxial and polycrystalline Pt is similar to the Ag/Pt and Ag/Pd cases, with large compressive coherency strain in the first few monolayers, followed by growth of relaxed Au. Surface morphology evolution, characterized by STM, clearly shows 2-D growth of strained Au, and 3-D growth of thick, relaxed Au. Lattice mismatch and surface energy differences are similar in the Ag/Pd, Ag/Pt and Au/Pt cases. Thus, the similarities in stress and microstructure evolution are consistent with the dependence of film growth behavior on fundamental quantities such as misfit strain, surface energies, and kinetic activation barriers.
[1]K. Bromann *et al.*, Phys. Rev. Lett. **75**, p 677, (1995).

11:45 AM O4.9
DISLOCATION ARRAYS IN THE INTERFACES BETWEEN SUBSTRATES AND EPITAXIAL ISLANDS. Annamalai Lakshmanan, Vidyut Gopal, Alex King, Eric Kvam, Purdue University, School of Materials Engineering, West Lafayette, IN.

A model to account for misfit dislocation array image effects during epilayer island growth is presented. Misfit dislocations often appear at an interface between phases to accommodate a lattice mismatch. In many situations, such as early film growth, one of the phases may be discontinuous, leaving the interface region clearly bounded. The structure of such a finite interface differs from the normally-modeled infinite interface because of end effects near the boundary. We have modeled the dislocation structure of such a finite interface, MBE-grown InAs on GaP, and compared our results to high resolution images of the same structure. The 11% misfit causes dislocation introduction from the outset of growth. Islands containing from 4 to 14 dislocations were examined, and dislocation spacings were found to be larger approaching the perimeter. Our calculations, which considered the image forces associated with the misfit dislocation array, model the observed structures well.

SESSION O5: EARLY STAGES OF FILM GROWTH: MECHANICAL PROPERTIES
Chairs: Steven M. George and Robert C. Cammarata
Wednesday Afternoon, April 18, 2001
Salon 7 (Marriott)

1:30 PM *O5.1
IMPACT OF NUCLEATION CONDITIONS ON TRANSFORMATION KINETICS AND MICROSTRUCTURE IN THIN-FILM SYSTEMS. J.M. Rickman, Dept. of MS&E, Lehigh University, Bethlehem, PA.

We examine quantitatively the impact of various nucleation conditions on the temporal evolution of a phase transformation, with particular emphasis on thin-film systems. Specifically, we characterize transformation kinetics and associated microstructures for catalyzed nucleation on crystalline defects and for cases in which there is a short-range interaction between nuclei. This is accomplished via the calculation of non-equilibrium, n-point correlation functions as well as related descriptors of spatial point processes using both computer simulation and complementary analytical work. One goal of this work is to relate both kinetics and microstructure to the underlying properties of the generating point process. Finally, in order to connect our models to experiment, we also discuss image processing strategies that have been employed to interpret relevant TEM micrographs.

2:00 PM O5.2
CORRELATIONS BETWEEN ISLAND NUCLEATION AND GRAIN GROWTH FOR POLYCRYSTALLINE FILMS.
C. Eisenmenger-Sittner, A. Bergauer, Institut für Angewandte und Technische Physik, Technische Universität Wien, Vienna, AUSTRIA.

For Physical Vapor Deposition (PVD) processes the nucleation and growth of stable islands on monocrystalline and even polycrystalline substrates can be described by the rate equation theory in a mean field approximation. The observable quantity which can be derived from the rate equations is the global density of stable islands. Interisland correlations and island size distributions, on the other hand, cannot be obtained from this formalism. The array of stable islands, in turn, forms the template for the subsequent growth of a polycrystalline thin film. For the initial grain shape and grain size therefore both, the global island density as well as possible interisland correlations play a key role. This paper presents the results of simulations which take into account the effects of both, the global island density as well as island/island correlations on the growth of a thick polycrystalline film. The simulations consist of two steps: first a polycrystalline template is generated from an initial distribution of stable islands by employing an algorithm for the construction of Voronoi-zones. The Voronoi zone network mimics the state of the film just after island coalescence and just before the onset of grain growth. Then the well known q-state Potts model of grain growth is employed to study the further steps of microstructural evolution. A higher initial island density leads to a faster onset of grain growth while a very homogenous distribution of islands significantly retards grain growth. The reasons for these effects are briefly discussed.

2:15 PM O5.3
MAGIC NANOSTRUCTURES DURING THE EARLY STAGE OF THIN FILM GROWTH. M. Zhang, M. Yu. Efremov, F. Schiettekatte, E.A. Olson, A.T. Kwan, J.T. Warren, R.S. Berry, J.E. Greene, and L.H. Allen, Dept of Materials Science and Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL.

The behavior of thin indium films at their early growth stage is

in-situ investigated by a novel ultra-sensitive thin film scanning calorimetry technique. These films consist of ensembles of indium nanostructures for which the melting temperature and latent heat of fusion are strongly influenced by their dimensions. We experimentally determine the relationship between the nanostructure radius and the melting point as well as the size effect on the latent heat of fusion by combining the measured caloric results with the nanostructure size distribution obtained from Transmission Electron Microscope studies. A linear melting point depression phenomenon is observed. More over, by looking at the fine structures of these caloric curves, the discrete nature of nanostructures has been revealed. The measured heat capacity values show several local maxima at certain temperatures. This suggests that preferred energy states exist among these self-assembled indium nanostructures on the amorphous surface during the early stage of thin film growth. These maxima relate to each other according to the nanostructure sizes by introducing one monolayer of indium atoms in thickness, which could be extended from the magic numbers observed previously in free cluster beams. (1) M.Y. Efremov, F. Schiettekatte, M. Zhang, E.A. Olson, A.T. Kwan, R.S. Berry and L.H. Allen, "Discrete periodic melting point observations for nanostructure ensemblems" Phys. Rev. Lett. 85, 3560 (2000) (2) M. Zhang, M.Y. Efremov, F. Schiettekatte, E.A. Olson, A.T. Kwan, L.S. Lai, J.E. Greene and L.H. Allen "Size-dependent melting point depression of nanostructures: Nanocalorimetric measurements" Phys. Rev. B., 62, 10548 (2000)

2:30 PM O5.4
NUCLEATION PHENOMENA AND MICROSTRUCTURE EVOLUTION OF VAN DER WAALS EPITAXY FILMS.
E. Wisotzki, A. Klein, W. Jaegermann, Materials Science Department Darmstadt University of Technology, Darmstadt, GERMANY.

(Quasi) Van der Waals epitaxy allows the epitaxial growth of lattice mismatched heterointerfaces. However, high quality films can only be expected when detrimental grain boundaries between different surface grains can be avoided. We have systematically investigated the growth of metals and 2-6 semiconductors on layered chalcogenide substrates with a systematic variation of substrate temperature and flux rate. The initial nucleation and subsequent film growth was studied by a combination of photoemission (XPS, UPS), electron diffraction (LEED) and scanning probe techniques (UHF-AFM/STM). The results show that different orientations of nucleation clusters are formed. Only some of them may intergrow to layer crystallites whereas others form grain boundaries at their contact area. The implications of these results for the perspective of (Quasi)-Van der Waals epitaxy for preparing interfacial buffer layers will be discussed.

3:15 PM *O5.5
DYNAMICS OF EULER BUCKLING INSTABILITY.
Leonardo Golubovic, West Virginia University, Department of Physics, Morgantown, WV.

Though Euler buckling instability of compressed thin objects is a classical subject, little is known on dynamical aspects that go with buckling phenomena. First deeper insights into buckling dynamics will be reviewed in this talk on the buckling dynamics of strained objects such as thin films and thin sheets (solid membranes). In recent simulations and analytical studies, we elucidated the very fundamentals of the dynamics of buckling phenomena in strained thin sheets and flexible rods. We related their buckling dynamics to that of the phase ordering phenomena such as the growth of ordered domains in magnetic systems below critical temperature [1]-[4]. Evolving thin sheets develop morphologies similar to that of growing interfaces, characterized by the presence of mounds with a size that grows as a power of time. Membrane morphology is characterized by the presence of a network of growing ridges where the elastic energy is mostly localized. We used this fact to develop a scaling theory of the buckling dynamics and deduce the coarsening exponents. Our findings have shown that the buckling dynamics constitutes a new class of coarsening phenomena characterized by novel scaling behaviors not found before in magnetic systems or elsewhere. [1] L. Golubovic, D. Moldovan, A. Peredera, Phys. Rev. Lett. 81, 3387 (1998). [2] D. Moldovan and L. Golubovic, Phys. Rev. Lett. 82, 2884 (1999). [3] D. Moldovan and L. Golubovic, Phys. Rev. E60, 4377 (1999). [4] L. Golubovic, D. Moldovan, and A. Peredera, Phys. Rev. E61, 1703 (2000).

3:45 PM O5.6
ELECTRON BEAM - DIRECTED VAPOR DEPOSITION OF MULTIFUNCTIONAL STRUCTURES. Douglas T. Queheillalt, Yash Katsumi and Haydn N.G. Wadley, Department of MS&E, School of Engineering and Applied Science, University of Virginia, Charlottesville, VA.

Multifunctional structures are those which combine load bearing support in addition to supplemental functions such as actuation, electrochemical energy storage or thermal management. Electron Beam - Directed Vapor Deposition (EB-DVD) technology has been used for the deposition of templated cellular structures and porous electrode coatings for rechargeable nickel - metal hydride cells. In addition to load bearing support, the templated cellular structures exhibit enhanced thermal management characteristics and the electrochemical cells can be integrated into the load bearing supports of linear and truss based structures leading to their multifunctionality. During EB-DVD, the electron beam evaporated vapor flux is encompassed by a rarefied transonic inert gas jet, entraining the vapor in a non-reactive gas flow and transporting it onto the current collector portion of the electrode structure. Here, EB-DVD technology has been used to synthesize Al and Cu based templated cellular structures for thermal management systems and porous nickel coatings for the positive electrode and porous rare earth (misch) metal coatings based on La and Ni (AB_5 alloys) or Ti and Zr (AB_2 alloys) for the negative electrode of rechargeable nickel - metal hydride cells.

4:00 PM O5.7
Transferred to O3.15

4:15 PM O5.8
NANOINDENTATION AND MICROSTRUCTURAL EVOLUTION STUDIES OF DC MAGNETRON SPUTTERED CHROMIUM NITRIDE THIN FILMS. Ankur B. Agarwal[a], B.A. Rainey[b], S.M. Yalisove and J.C. Bilello, Center for Nanomaterials Science, Department of MS&E, University of Michigan, Ann Arbor, MI. [a]Now at Advanced Micro Devices, Sunnyvale, CA. [b]Now at IBM, Burlington, VT.

Nanoindentation experiments have been performed to assess the mechanical behavior of chromium nitride (Cr_xN_y) thin films sputtered in different deposition geometries and with varying Ar and N_2 pressures. The hardness and elastic modulus of chromium nitrides are of great interest with regard to their applications. In the present work, two different deposition geometries, i.e. multi-substrate and confocal, were used to sputter (DC magnetron) a Cr_xN_y layer on Si (100) wafers at varying nitrogen flow rates. The results of the nanoindentation experiments indicate that, over a similar argon and nitrogen regime, the Cr_xN_y films grown in a multi-substrate geometry exhibit higher hardness and elastic modulus on the average than those grown in the confocal geometry. Furthermore, it was found that in the multi-substrate geometry the hardness and elastic modulus of the films were significantly higher than those in the confocally deposited films for a specific regime of the nitrogen flow rate (10-14 sccm). Finally, observations of the mechanical properties trends could be correlated with a higher degree of anisotropic stress for films grown in the multi-substrate in comparison to the confocal geometry.

4:30 PM O5.9
FRICTION AND WEAR BEHAVIOR OF Al-Cu-Fe-B QUASICRYSTAL. Xiying Zhou, Dept of Materials and Science, Nanchang Institute of Aeronautical and Technology, Nanchang, CHINA; Caroline Richard, Dept of Materials, Univ of Technology of Compiegne, Compiegne, FRANCE.

Dry sliding wear between the polycrystalline Al59Cu25.5Fe12.5B3 quasicrystals and coating of the Diamond-Like Carbon (DLC) is carried out by self-made tribometer under different conditions. The influences of four parameters (temperature, sliding speed, applied loading, the atmosphere) on friction and wear of quasicrystal surface are studied. In addition, the surface microstructure and the morphology have been observed by scanning electron microscopy (SEM) and X-ray diffraction. The results show that, with rise of the applied load and sliding speed, the friction coefficient decreases. The friction coefficient is influenced greatly by the temperature and increased evidently by the rise of temperature. Analyze of the wear mechanism illustrates that not only abrasive wear but also adhesive wear exist in surface of the quasicrystals. At 350°, delaminating mechanism is main wear mechanism for quasicrystal. Moreover, Analyze of the surface morphology illustrates that the microcracks sub-crack (or second crack) form, to different extent, in all worn quasicrystal surface. All discussion and analyses on the results of experiment are presented in detail. Keywords: Quasicrystal, Temperature, Friction coefficient, Microcrack

SESSION O6: TEXTURE IN POLYCRYSTALLINE FILMS
Chairs: Leonardo Golubovic and David L. Windt
Thursday Morning, April 19, 2001
Salon 7 (Marriott)

8:30 AM *O6.1
MATHEMATICAL MODELS OF ION BEAM ASSISTED DEPOSITION OF MgO. Peter Smereka, Dept. of Mathematics, University of Michigan, Ann Arbor, MI.

One of the promising approaches to a producing superconducting tape using YBCO is to deposit the YBCO onto a MgO substrate. Typically a MgO substrate will be a polycrystalline film with a (001) fiber texture. However, to obtain a high quality superconducting tape it has been determined that one needs MgO films with good in-plane texture. One successful approach is to use ion beam assisted deposition(IBAD) of MgO. This has resulted films with excellent in-plane texture. This talk will describe mathematical models for this problem and for other problems involving growth of polycrystals. The first part of the talk will describe the computation of polycrystals using narrow band level set methods. Computations of IBAD MgO will then be presented. We still need to explore various models of IBAD MgO and the level set approach is, unfortunately, too slow to compute models of IBAD MgO growth with a large number of crystals. For this reason, a simplified computational strategy has been developed which allows for the approximate solution of the mathematical model for IBAD MgO. The results of the simplified approach show that two of the key parameters controlling the in-plane texture are the seed nucleation density and the out-of-plane texture. The model shows that there is an optimal film thickness, after which the in-plane texture will not improve and the surface roughness increases. Furthermore, the MgO surface appears to tilt toward the ion beam. The predictions of the in-plane texture are in reasonable agreement with experiments as is the optimal film thickness. (This is joint work with G. Russo, X. Li, and D. Srolovitz)

9:00 AM O6.2
IN SITU BIAXIAL TEXTURE ANALYSIS OF MgO FILMS DURING GROWTH ON AMORPHOUS SUBSTRATES BY ION BEAM-ASSISTED DEPOSITION. Rhett T. Brewer[a] Paul N. Arendt[b], James R. Groves[b], and Harry A. Atwater[a], [a]California Institute of Technology, Dept of Applied Physics, Pasadena, CA; [b]Los Alamos National Laboratories, Los Alamos, NM.

Ion beam-assisted deposition (IBAD) has been demonstrated to produce biaxially textured thin films on amorphous substrates. Magnesium Oxide is particularly interesting because its biaxial texture is optimally developed within the first 11 nm of growth and single crystal MgO has already been studied as a heteroepitaxial template for ferroelectrics and superconductors. However, obtaining experimental evidence to examine the biaxial texturing mechanisms of IBAD MgO has been difficult due to the *ex situ* nature of conventional biaxial texture analysis techniques and the difficulties associated with studying thin films of MgO with X-rays. We used a previously reported RHEED based method for performing quantitative analysis of mosaic polycrystalline thin film in-plane and out of plain grain orientation distributions to make *in situ* biaxial texture measurements of IBAD MgO. RHEED in-plane rocking curve analysis of IBAD MgO films, at 25 keV and 2.7° incidence angle, measures in-plane orientation distributions on the order of 4° to 5° narrower than measured using X-ray rocking curve analysis or transmission electron microscopy (TEM). Because biaxial texture typically improves with film thickness during IBAD, these measurements indicate that RHEED in-plane rocking curves offer better surface sensitivity than X-ray diffraction for analyzing film in-plane orientation distributions. RHEED is sensitive to films as thin as 30 angstroms, allowing us to sequentially observe the biaxial texture from just after grain nucleation, through island growth, film coalescence, and complete coverage growth. The degree of biaxial texturing accomplished during nucleation and the rate of biaxial texture evolution before film coalescence (when ion-induced anisotropic sputtering is most important), as well as after film coalescence (when both ion-induced anisotropic grain damage and sputtering can improve biaxial texture) will be discussed.

9:15 AM O6.3
PHASE FIELD SIMULATIONS OF OBLIQUE INCIDENCE BALLISTIC DEPOSITION. Markus Rauscher, James P. Sethna, Cornell University, Physics Dept, Ithaca, NY; Liguo Wang, Paulette Clancy, Cornell University, Dept of Chemical Engineering, Ithaca, NY.

Recent developments in energetic beam deposition techniques allow to deposit metals and semiconductors on surfaces with controlled energy and incident angle. For oblique incidence, formation of columnar structures has been observed experimentally as well as in Kinetic Monte Carlo (KMC) simulations. We study the growth of these structures in a continuum phase field model, to overcome the limitations of KMC. Our model includes shadowing, anisotropic surface tension, and angle dependent sticking rates. We study the growth angle and coarsening behavior as a function of the incident angle and compare our simulations results with experiments and KMC simulations.

9:30 AM O6.4
HIGH FLUX, LOW-ENERGY ION BOMBARDMENT ENHANCED CRYSTALLINITY OF POLYCRYSTALLINE Si THIN FILMS. Jennifer E. Gerbi, John R. Abelson, University of Illinois at Urbana-Champaign and Coordinated Science Laboratory, Urbana, IL.

We deposit polycrystalline silicon films at low temperatures (400C) on glass using magnetron sputtering at low pressures. Using an external magnetic field, we unbalance the magnetron, increasing the ion/neutral flux ratio while limiting the ion energy via substrate bias to $\sim$20eV; this energy is large enough to promote adspecies motion but is too small to produce sub-surface point defects. Using Raman scattering, ellipsometry, TEM, and AFM, we show that this shower of low energy, high flux ions increases the grain size of thin films (e.g., from 40nm to 100nm for 400nm thick films) while keeping the films extremely smooth (1.9nm rms surface roughness). The thickness of the interface layer of amorphous film that exists before the polycrystalline Si nucleates is also strongly decreased, indicating that nucleation barriers are reduced. The mechanism by which the ions enhance crystalline growth is studied here by performing two experiments using in-situ, fully spectroscopic, fast ellipsometry. Ion-enhanced epitaxy experiments are performed on Si substrates to probe the epitaxial thickness and quality as a function of arriving ion flux and energy. Additionally, growth is performed on intentionally rough substrates, and the rate of smoothening is measured as a function of ion flux. We interpret both results in terms of ion bombardment enhanced adatom diffusion, and discuss the mechanistic implications for direct deposition of polycrystalline Si at low temperatures.

9:45 AM O6.5
ATOMISTIC MODELS OF THE DEPOSITION OF Cu AND Al THIN FILMS FOR INTERCONNECT APPLICATIONS. J. Dalla Torre, G.H. Gilmer, F.H. Baumann, P.L. O'Sullivan, Bell Laboratories, Lucent Technologies, Murray Hill, NJ.

The sputter deposition of Al and Cu onto a foreign substrate usually results in 3D island nucleation and, eventually, coalescence into a polycrystalline film. The relatively high diffusivity of these materials permits the transport of deposited material across the substrate, and transfer between islands, so as to reduce the total of the surface, interfacial and bulk strain free energy. The Al and Cu films used in Si device metallization are examples of this process, since the Al conductor layers are usually deposited by sputtering, as well as the Cu seed layers. There are problems with the formation of voids in Al films during deposition, primarily as the islands coalesce, and with the incomplete coverage of the barrier layer films by the Cu seed layer. Voids can act as preferred sites for electromigration, and for de-wetting of the film from the substrate during annealing. We have developed Monte Carlo simulations to study island growth and coalescence during deposition, and to predict the resulting microstructure of the films, including voids and grain boundaries. These simulations give the thickness at which island merger occurs, and thus the minimum thickness required for the formation of a continuous film. We have developed an analytical model of island growth in order to provide fast estimates of coverage and film quality, using Monte Carlo simulations only to test the applicability of the analytical model to different conditions of film growth. We have also applied the Monte Carlo simulations to study the influence of various deposition techniques on the structure of the films. We have examined the influence of energetic beams on the nucleation and merger of clusters, as well as that of cluster beams. Results for the simulations are validated using sputter deposition experiments, including magnetron sputtering systems similar to those used in the fabrication of Si devices.

10:30 AM *O6.6
MULTISCALE MODELLING OF GROWTH OF POLY-CRYSTALLINE THIN FILMS. James B. Adams, Jie Zhang, Zhiyong Wang, Arizona State University, Dept of Chemical and Materials Engineering, Tempe, AZ.

We have developed two new modelling tools for studying the growth of polycrystalline thin films, POLYGROW and FACET. POLYGROW is a 3D polycrystalline kinetic lattice Monte Carlo code that can simulate the deposition of BCC metals for long times. It is based on a knowledge of the atomic-scale thermodynamics and kinetics of film growth. We will present results for the deposition of Mo tips, the effect of chemical etching, and the effect of long-term annealing on the tip structure. FACET is a 2D simulation of polycrystalline film growth on the micron scale. It models films in terms of individual grains, with each grain having its own orientation, surface facets, and grain boundaries. It includes both deposition and surface diffusion events, with surface diffusion rates calculated by a 3D and/or 1D KLMC atomic model. This code allows one to easily visualize the evolution of grain morphology during film growth in real time. We will present several results relating to PVD of Cu.

11:00 AM O6.7
CORRELATION BETWEEN SURFACE AND MICROSTRUCTURE EVOLUTION IN MBE DEPOSITED Al FILMS ON Si (111) AND

SiO_2. Adriana E. Lita, Lucent Technologies, Reading, PA; Catalina Dorin and Joanna Mirecki-Millunchick, Dept. Materials Science and Engineering, Univ. Michigan, Ann Arbor, MI; John Sanchez, Jr., Advanced Micro Devices, Sunnyvale, CA.

We have investigated the role of grain boundaries and microstructure on surface profile evolution in MBE deposited Al films on Si (111) and SiO_2 substrates. The growth of Al films from 5 nm and 500 nm in thickness at 0.04 nm/sec and 0.15 nm/sec and 50 C was monitored by in-situ RHEED. Post-deposition characterization included plan view and cross-section transmission electron microscopy (XTEM),atomic force microscopy coupled with power spectral density (1DPSD) analysis, and x-ray pole figure analysis. Characteristic dimension (CD) length scales indicative of feature size on the growing Al surfaces were determined by the 1DPSD methodology. While the CD increases monotonically with thickness for the Al on SiO_2, the CD increase is markedly reduced at about 50 nm Al thickness on Si (111), concurrent with a significant increase in the temporal roughness exponent (β). Plan view EM and the Al (111) x-ray pole figures indicate that the Al is pseudo-single crystalline on the Si (111), consisting of Al (111) out-of-plane oriented domains with Al $<220>$ slightly misoriented ± 7 degrees from Si $<220>$ along the substrate surface. Interestingly, only one Al (111)/Si (111) variant ("A") was observed by pole figure analysis until approx. 100 nm Al thickness, at which time the "B" variant emerged. Significantly, a new Al (200) texture component emerges at 200 nm thickness, consistent with faceted grains revealed by XTEM which have formed at the growing Al surface. The surface and microstructural evolution in the MBE deposited Al films on SiO_2 was consistent with previously reported Al sputter depositions on SiO_2. Correlation between the surface profile evolution and texture and microstructure effects as well as surface mechanisms which possibly generate novel texture components are discussed.

11:15 AM O6.8
TEXTURE EVOLUTION IN Al(Cu) INTERCONNECT MATERIALS. Conal E. Murray and Kenneth P. Rodbell, IBM T.J. Watson Research Center, Yorktown Heights, NY.

An investigation of the microstructural evolution of Al(Cu) thin films deposited on a variety of interlevel dielectric (ILD) layers was performed. A combination of X-ray texture measurements and scanning electron microscopy (SEM) was employed to link the texture behavior of the as-deposited Al(Cu) films at different thicknesses to the observed morphological development within the films. Three regimes of texture were revealed, corresponding to (1): Al(Cu) island growth and individual island coalescence, (2): fully coalesced film and the onset of grain growth and (3): extensive grain growth. The first and last of these regimes exhibited offset (111) texture, in which the maximum diffracted intensity from Al (111) is offset from the substrate normal. However, the position of maximum offset texture differed between the two stages of growth, indicating that two different mechanisms were responsible. The offset (111) texture observed in the third regime of Al(Cu) film microstructure was due to the faceting of grain surfaces. The time required for the films to reach these three stages depended on the effective diffusivity of the Al adatoms on the ILD surfaces, which differed in chemistry and topography. Because research on Al(Cu)/Ti/ILD structures revealed a dependence of the offset (111) texture on ILD surface morphology, a link between the remnants of island growth in the Al(Cu) films deposited directly onto ILD's and their subsequent grain orientations during the final growth stage will be discussed.
[1]C.E. Murray and K.P. Rodbell, "Texture Inheritance in Al(Cu) Interconnect Materials", J. Appl. Phys., in press.

11:30 AM O6.9
CONTINUUM MODELS OF SPUTTER DEPOSITION INCORPORATING FINITE ATOMIC LENGTH SCALES. P.L. O'Sullivan, G.H. Gilmer, F.H. Baumann, J. Dalla Torre, Bell Laboratories, Lucent Technologies, Murray Hill, NJ; C.-S. Shin, I. Petrov and T.-Y. Lee, Materials Research Laboratory, University of Illinois, Urbana, IL.

We investigate a limitation of the continuum model of thin film deposition over sharp-cornered features by comparing numerical simulations with experiments on the sputter deposition of Ta. Our work is relevant to the accurate prediction of step coverage for barrier and seed layers deposited using physical vapor deposition. The physics of non-local interactions due to the finite atomic size causes atoms to be captured by the film, even at grazing incidence, resulting in "breadloafing" at sharp convex corners. That is, atoms that fall within the capture range of a vertical sidewall of a trench, for example, will stick on the sidewall and cause the film to advance laterally at that point. This effect does not vanish as the size of the atoms shrinks to zero, since the lateral advance is proportional to that in the vertical direction, the layer thickness, and both are proportional to the atomic radius. An atomistic model based on a lattice Monte Carlo method shows the characteristic breadloafing at the upper corners of a trench, extending outward at an angle comparable with that observed in the experiment. Conversely, the continuum model does not produce overgrowth since there is no mechanism for it: mathematically, the film should grow purely in the vertical direction in the case of a collimated, vertical flux. The main idea for incorporating this key feature of the atomistic model into the continuum model is to calculate the flux to sections of the film using a capture zone that surrounds the actual film surface. Films simulated using this mechanism exhibit overgrowth at the edge of a trench, and as the film grows the two overhangs impinge and merge leaving a void in the trench. Additional details and results will be presented.

11:45 AM O6.10
SYNTHESIS AND PROPERTIES OF Al-BASED AMORPHOUS AND MICROCRYSTALLINE THIN FILMS. L. Berger, J. Mrosk and H.-J. Fecht, Ulm University, Center for Micromaterials, Ulm, GERMANY.

Thin films of Al-based alloys have been produced by ultra-high vacuum electron beam co-evaporation. The properties of the films with a thickness up to 400 nm have been further characterized by x-ray and electron diffraction, AFM, nanoindentation and electrical resistance measurements using samples as deposited and annealed at different temperatures. Amorphous Al-14at%Y films are found to be particularly suitable for applications in surface acoustic wave devices (SAW) due to their high mechanical strength of about 1.3 GPa and their atomistically smooth surfaces when compared with conventional polycrystalline Al-based metallizations.

SESSION O7: GRAIN GROWTH: BARRIER LAYERS
Chairs: Peter Smereka and James B. Adams
Thursday Afternoon, April 19, 2001
Salon 7 (Marriott)

1:30 PM O7.1
SURFACE BOUNDARY AND TRIPLE JUNCTION EFFECTS DURING GRAIN GROWTH IN POLYCRYSTALLINE FILMS. Amanda L. Giermann, Dept of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL; Elizabeth A. Holm, Materials Theory and Computation, Sandia National Laboratories, Albuquerque, NM; Alexander H. King, Rachel E. Cefalu, School of Materials Science and Engineering, Purdue University, West Lafayette, IN.

Grain growth in polycrystalline films commonly ceases when the mean grain diameter is approximately equal to the film thickness. Three-dimensional Monte Carlo grain growth simulations were used to explore three proposed mechanisms for this stagnation: grain boundary grooving, triple junction drag, and low triple junction free energy. When surface boundaries have a lower mobility than bulk boundaries due to grain boundary grooving, grain growth slows but does not stop, nor do the catenoidal grains, abnormal triple junction angles, or atypical grain size distributions predicted by theory occur. If reduced triple junction mobility causes triple junction drag, grain vertex angles deviate from 120 degrees and the grain size distribution narrows, but the total curvature per grain boundary, thus the driving force for growth, remains constant. Therefore, while growth kinetics decrease, stagnation again does not occur. When triple junctions have a negative free energy relative to grain boundaries (as proposed by King [1]), three regimes are observed. For the lowest triple junction energies, the system disorders. For high triple junction energies, normal growth occurs. For moderate triple junction energies, three-dimensional systems disorder, but columnar (two-dimensional) polycrystals grow normally. In no case is stagnation observed. These results are compared to experimental observations using a new method for measuring boundary curvature. Alternate causes for grain stagnation are proposed. [1] A.H. King, Interface Science 7 (1999) 251-271.

1:45 PM O7.2
COUPLING OF THERMAL GROOVING AND MIGRATION OF INCLINED GRAIN BOUNDARIES. Huifang Zhang, Harris Wong, Louisiana State Univ, Dept of Mechanical Engineering, Baton Rouge, LA.

Grain boundary migration is a fundamental process governing grain growth. The motion of a grain boundary is significantly affected by the presence of a free surface because of the formation of a groove at the triple junction. The interaction of grain boundary migration and thermal grooving has not been studied in detail. We have coupled thermal grooving and grain-boundary migration for slightly inclined grain boundaries, and obtained free-surface and grain-boundary profiles. We assume that thermal grooving results from surface diffusion whereas grain boundary migration obeys a curvature-driven law of motion. A range of length and time scales are needed to

describe the coupled motion. It is found that the grain boundary is never pinned. We will present these results and discuss the implications.

2:00 PM O7.3
ROLE OF SUBSTRATE AND GROWTH PROCESSES ON TEXTURE EVOLUTION IN VAPOR DEPOSITED Al AND Cu THIN FILMS. John Sanchez Jr., Advanced Micro Devices, Sunnyvale, CA; Adriana E. Lita, Lucent Technologies, Reading, PA.

Successful strategies for controlling the microstructure of vapor deposited thin films include proper choice of substrate or barrier materials. However understanding of the various mechanisms responsible for microstructure control by the substrate is incomplete. We present the characterization of sputter deposited Al and Cu thin films from 10 nm to greater than 1000 nm in thickness on SiO_2, Ti and Ta layers by x-ray pole figure, atomic force microscopy and cross-section transmission electron microscopy. The 10 nm thick Al films on SiO_2 and Ti and 10 nm Cu film on Ta are primarily randomly oriented. However the 10 nm Al on SiO_2 is discontinuous and consists of both faceted and rounded islands. We show that the faceted islands are larger than average size and are oriented approx. 5 degrees from exact fiber orientation, whereas the rounded islands are randomly oriented. Upon achieving film continuity these larger/faceted/5 degree tilted Al grains promote the evolution of the near Al (111) 5 degree film texture characteristic of Al films on SiO_2. In contrast the 10 nm Al on Ti is continuous, and an exact Al (111) fiber texture emerges as a result of normal and abnormal grain growth concurrent with continued deposition. Similarly, the texture of 10 nm thick Cu films on Ta are also primarily randomly oriented, with the exact Cu (111) fiber texture evolving as grain growth and deposition proceed. We conclude by discussing the combination of island stage growth mechanisms, abnormal and normal grain growth processes and substrate effects as microstructure develops during deposition.

2:15 PM O7.4
IN SITU X-RAY MEASUREMENTS OF TEXTURE EVOLUTION DURING ANNEALING OF METALLIC THIN FILMS. J.A. Floro, J.A. Hunter, Sandia National Laboratories, Albuquerque, NM; E. Chason, Div. of Engineering, Brown University.

Texture evolution in polycrystalline thin films is a direct result of processes occurring both during the nucleation stage of film growth, and during recrystallization or grain growth in continuous films. We will present preliminary measurements of texture evolution in Ag and Al thin films using a new in situ x-ray diffraction capability. In this talk we will discuss the real-time evolution of (111) and (001) fiber textures during annealing of Ag and Al films, and correlate texture evolution with grain growth. When Ag is deposited at temperatures in the range -50 to -80°C, and then warmed to room temperature and above, texture development exhibits a sharp onset near -10°C, for films with thicknesses that vary by an order of magnitude. By contrast, Al films deposited under similar conditions exhibit a continuous development of texture with temperature. For Ag films, a competition between (111) and (001) textures is observed, with the preference for (001) increasing with increasing film thickness. Only (111) texture is observed in Al films. The x-ray data also contains information on the variation of the out-of-plane lattice parameter with temperature for both the (111) and (200) texture components. These results will be interpreted within a framework of orientation-specific grain growth that minimizes both surface and elastic energy. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

2:30 PM O7.5
MICROSTRUCTURAL COMPARISON OF Ag FILMS GROWN ON AMORPHOUS TiO_2 AND POLYCRYSTALLINE ZnO.
Rand Dannenberg, Darin Glenn, AFG Development Corporation, Petaluma, CA; E.A. Stach, National Center for Electron Microscopy, Lawrence Berkeley Lab, Berkeley, CA.

16 nm Ag films were sputter deposited onto amorphous TiO_2 underlayers 25 nm thick, and also amorphous TiO_2 (25 nm)/ZnO (5 nm) multi-underlayers. The substrates were back-etched Si with a 50 nm thick LPCVD Si_3N_4 electron transparent membrane. The ZnO, sputtered onto amorphous TiO_2, formed a continuous layer with a grain size of 5 nm in diameter, on the order of the film thickness. There are several microstructural differences in the Ag dependent on the underlayers, revealed by TEM. First, on TiO2 the Ag microstructure shows many abnormal grains whose average diameter is about 60-80 nm, whereas the films on ZnO show few abnormal grains. The background matrix of normal grains on the TiO_2 is roughly 15 nm, while the normal grain size on the ZnO is about 25 nm. Electron diffraction patterns show that the film on ZnO has a strong {111} orientation, and dark field images with this diffraction condition have a grain size of about 30 nm. In a region near the center of the TEM grid where there is the greatest local heating during deposition, Ag films grown on amorphous TiO_2 are discontinuous, whereas on ZnO, the film is continuous. When films are grown on solid glass substrates, those with ZnO underlayers have sheet resistances of 5.68 ohm, whereas those on TiO_2 are 7.56 ohm. The conductivity difference is very repeatable. The improved conductivity is thought to be a combined effect of reduced grain boundary area per unit volume, the predominance of low grain boundary resistivity Coincidence Site Lattice boundaries from the {111} orientation, and Ag planarization on ZnO resulting in less groove formation on deposition.

2:45 PM O7.6
INFLUENCE OF THE SPUTTERING GAS ON THE PREFERRED ORIENTATION OF NANOCRYSTALLINE TITANIUM NITRIDE THIN FILMS. Rajarshi Banerjee, Gregory B. Thompson, Hamish L. Fraser, Dept of MS&E, Ohio State University, Columbus, OH; Ramesh Chandra, Dept of Physics, Guru Nanak Dev University, Amritsar, INDIA; Pushan Ayyub, Dept of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai, INDIA.

Titanium nitride thin films have a wide variety of applications both for structural as well as electronic applications. Their hardness makes them ideal candidates for wear resistant applications. In addition, the excellent electrical conductivity of titanium nitride combined with the fact that it is a good diffusion barrier makes it an excellent contact material in the microelectronics industry. Nanocrystalline titanium nitride thin films have been deposited by high pressure reactive magnetron sputtering from an elemental titanium target using a mixture of an inert gas and nitrogen. The mean crystallite or grain size in these films is in the range 9-12 nm as measured from the Debye-Scherrer line broadening in the x-ray diffraction patterns. Interestingly, the type of inert gas used in the sputtering gas mixture significantly influences the preferred orientation of growth in these films. Thus, using a helium and nitrogen gas mixture results in a strongly {002} oriented film whereas using a argon and nitrogen gas mixture results in a strongly {111} oriented film. In addition, films have also been deposited using pure nitrogen as the sputtering gas. The films deposited using pure nitrogen exhibited a strong {002} orientation and had a significantly larger grain size as compared with those deposited using a mixture of an inert gas and nitrogen. Details of the microstructural evolution in these films based on characterization using transmission electron microscopy will be discussed in this paper. The ability to tailor the size of crystallites and their preferred orientation in these films is expected to have a significant impact on their properties for a variety of technological applications.

3:30 PM *O7.7
NUCLEATION AND GROWTH DURING TUNGSTEN ATOMIC LAYER DEPOSITION ON OXIDE SURFACES. S.M. George, J.W. Elam, R.K. Grubbs, J.W. Klaus and C.E. Nelson, Dept. of Chemistry and Biochemistry, University of Colorado, Boulder, CO.

Tungsten atomic layer deposition (ALD) can be accomplished by separating the binary reaction $WF_6 + Si_2H_6 \rightarrow W + 2SiHF_3 + 2H_2$ into two self-limiting half-reactions. Successive exposure to WF_6 and Si_2H_6 in an ABAB... sequence has produced W ALD at a rate of 2.5 Å per AB cycle at 425 K. The nucleation and growth during W ALD on oxide surfaces have been studied using Auger electron spectroscopy (AES). The AES results displayed an initial nucleation period of 7-8 AB cycles to deposit one tungsten monolayer on SiO_2. The W and Si AES signals grew and oscillated dramatically versus WF_6 and Si_2H_6 exposures. An examination of the oxygen and tungsten AES signals versus AB cycles indicated that W ALD displayed nearly ideal layer-by-layer, Frank van der Merwe growth after the nucleation period. The AES results displayed a shorter nucleation period of 3-4 AB cycles for W ALD on Al_2O_3. The W and Si AES signals again oscillated versus WF_6 and Si_2H_6 exposures. However, the oxygen and tungsten AES signals versus AB cycles showed that W ALD did not completely wet the underlying Al_2O_3 surface. The W ALD was consistent with Stranski-Krastanov or Volmer-Weber growth with tungsten covering ~95% of the Al_2O_3 surface. The initial nucleation period during ALD is important because the number of AB cycles required for nucleation can affect the roughness of the resulting ALD films.

4:00 PM O7.8
COMPARISON STUDY FOR TiN FILM DEPOSITED FROM DIFFERENT METHOD: CHEMICAL VAPOR DEPOSITION AND ATOMIC LAYER DEPOSITION. Byoung Youp Kim, Sung Hyun Lee, Ki Young Oh and Juho Song, Jusung Engineering Limited, Kyung Ki Do, KOREA.

Recent advanced semiconductor devices require metal barrier processes of low process temperature and excellent film step coverage without the degradation of resistivity and impurity content level in

the film. This paper compared two different film deposition processes for formation of TiN barrier layers, conventional TiCl4-based chemical vapor deposition and atomic layer deposition(ALD). The 300Å thick TiN films deposited by conventional TiCl4-based CVD at the process temperature of 600°C followed by NH3 post-deposition anneal showed about 180$\mu\Omega$·cm of resistivity, over 95% of step coverage for the pattern aspect ratio of 7 on 0.3μm contact diameters, and below 2 at.% of Cl contents in the film. Meanwhile, the films deposited by ALD at 100°C lower process temperature than CVD even without post-deposition anneal showed much better film properties which were almost the same resistivity values along with better step coverage characteristics. More detailed material analysis was done by AFM, XPS, SEM, and AES. Studies of film growth processing parameters such as process temperature, reaction gas ratio, chamber pressure, post-deposition anneal for both methods and analysis results would be included.

4:15 PM O7.9
Abstract Withdrawn.

4:30 PM O7.10
NANOSCALE TEXTURE DETERMINATION AND EVOLUTION IN ULTRA-THIN TiN FILMS. Mark J. Williamson, Derren Dunn, Robert Hull, University of Virginia, Department of MS&E, Charlottesville, VA; Suneel Kodambaka, Ivan Petrov, Joe Greene, University of Illinois, Department of Materials Science, Urbana, IL.

As the feature size of devices in integrated circuits continues to shrink there is a need to characterize polycrystalline materials on decreasing length scales. For example, it is necessary to develop ultra-thin diffusion barriers for interconnect structures, and a critical part of this development is to ensure that these barrier materials have the optimum grain structure and texture. We will present results on the texture evolution and grain morphology in fine-grained TiN thin films. In order to do this we have developed a technique using cross-correlation of dark-field images obtained using annular objective apertures in the transmission electron microscope, with annuli radii that correspond to the low index TiN reflections. This technique enables parallel analysis of the orientations of thousands of grains, with a spatial resolution of order 10 nm. This combination of spatial resolution and high throughput is not possible with x-ray diffraction, electron backscattered diffraction or conventional transmission electron microscopy. Preferred grain orientations were determined for 40-, 60-, 80- and 100-nm-thick TiN layers grown on amorphous SiO_2 at 400 °C by magnetically-unbalanced reactive magnetron sputter deposition. We find that no single orientation is dominant in the 40 nm films but that a $< 100 >$ texture develops and continues to grow by the time these films reach 60 nm in thickness. These results demonstrate that in ultra-thin diffusion barriers, processing conditions will have to be carefully understood and designed to ensure optimum microstructures.

4:45 PM O7.11
EFFECT OF RAPID-THERMAL-ANNEALING ON TIN FILMS AS THE BARRIER LAYER FOR THE Pt/BST/Pt CAPACITORS PREPARED BY RF MAGNETRON CO-SPUTTER TECHNIQUE AT LOW TEMPERATURE. Miin-Horng Juang, National Taiwan University of Science and Technology, Dept. of Electronic Engr, Taipei, TAIWAN; Chuan-chou Hwang, Huang-Chung Cheng, National Chiao-Tung University, Dept. of Electronics Eng., Hsin-chu, TAIWAN.

Thin barium strontium titanate (BST) film with a high dielectric constant has attracted much attention for practical use in high-density DRAM capacitors. In the capacitors of capacitor-over-bit-line (COB) structure, a diffusion barrier of TiN is often used to prevent the electrode and dielectrics from chemical reaction with poly-Si plug and TiN adhesion layer during BST deposition and post processes. In this study, the Pt/BST/Pt/TiN/Ti/Si structure is used to simulate the practical COB capacitor structure. Effect of rapid thermal annealing on metallic barrier TiN against the interdiffusion of Ti and Si into BST has been investigated. In the integration of BST capacitors, the thermal budget of the BST deposition would cause the interdiffusion of Ti and Si from Ti adhesion layer and poly-Si plug respectively. This event would degrade the BST capacitors. To address this issue, rapid-thermal-annealed TiN barrier was deposited between the bottom electrode Pt and the adhesion layer Ti. By RTA-treating the TiN barrier layer, good barrier properties were achieved. The RTA treatment at 600°C for 90 sec can improve the crystallinity of TiN and suppress the formation of unexpected materials. Excellent electrical characteristics of the Pt/BST/Pt/TiN/Ti/Si capacitors, including a high dielectric constant of 320, a low leakage current of 15 nA/cm^2 under 0.1 MV/cm, and a lifetime longer than 10 years under 1.6 MV/cm were obtained for the BST films formed by uisng co-sputtering with an Ar O_2 mixed ambient at a low substrate temperature of 300°C. On the other hand, the TiN barrier was not suited for excessively elevated RTA temperature above 700°C. Owing to high roughness asperity of the Pt/TiN surface formed during the RTA treatment at 700°C, the leakage current increased significantly and dielectric degradation was thereby accelerated.

SESSION O8: POSTER SESSION
Chairs: John E. Sanchez and George H. Gilmer
Thursday Evening, April 19, 2001
8:00 PM
Salon 1-7 (Marriott)

O8.1
MODELLING OF GALLIUM NITRIDE GROWTH FROM TRIMETHYL GALLIUM AND AMMONIA: REACTION PATHWAYS AND RATES. Debasis Sengupta, Sandip Mazumder, CFD Research Corporation, Huntsville, AL.

Reactor scale modeling of chemical vapor deposition has recently drawn much attention due to its potential for cost effective development of next generation solid-state devices. The most challenging aspect of the large-scale reactor modeling is the accurate determination of the rate constants of reactions occurring between the precursors, both in the gas phase and at the surfaces. The predictive ability of reactor modeling is limited by the accuracy of the rate constants used for gas phase reactions and the reactions at the surface. Over the last few years, Gallium Nitride has attracted significant attention due to its ability to produce blue light, and wide band-gap transistors. This article presents a "first principles" approach to the calculation of the reaction rates for gas phase and surface reactions occurring during MOVPE of Gallium nitride using trimethylgallium and ammonia as precursors. Our approach uses fundamental concepts of statistical mechanics, transition state theory in conjunction with ab initio quantum chemistry method to calculate surface reaction rate constants. The gas phase rate constants were calculated as a function of temperature and pressure by combining quantum chemical method with the quantum RRK (QRRK) theory. To calculate the pre-exponential factors for adsorption and desorption reactions of various gas phase species, a loose transition state is assumed where the adsorbate moves over the surface with a two-dimensional translational motion. Moreover, the appropriate degrees of freedom have been assigned for the adsorbates at the gas phase, transition states for adsorption and adsorbed states in order to calculate the pre-exponential factor accurately. The activation barriers for surface reactions were either extrapolated from the analogous gas phase reactions or calculated using a cluster model. Calculated rate constants were then used for commercial reactor scale modeling of gallium nitride deposition. Modeling results exhibit excellent match with available experimental data.

O8.2
THE EFFECTS OF INTERRUPTION TIME ON HIGH In CONTENT InGaN/GaN QUANTUM WELL GROWN BY METALORGANIC CHEMICAL VAPOR DEPOSITION.
M.G. Cheong, C.S. Kim, R.J. Choi, Y.K. Hong, H.S. Yoon, S.W. Yu, C.-H. Hong, E.-K. Suh and H.J. Lee Semiconductor Physics Research Center and Department of Semiconductor Science and Technology, Chonbuk National University, Chonju, KOREA; H.K. Cho and J.Y. Lee Department of MS&E , Korea Advanced Institute of Science and Technology, Taejon, KOREA.

In recent years, InGaN/GaN multi quantum wells (MQWs) have received much attention as the active material in blue and green light emitting diodes (LEDs) and light diodes (LDs). However, despite the remarkable progress in device performance, comprehension of InGaN/GaN QW is still a vigorous research field. The compositional fluctuation of In and V-defects in InGaN/GaN QW have been studied about their roles and origins by many groups. It has been controversial that the luminescence center in InGaN QW is originated from the presence of In rich region or the self-formation of quantum dot (QD) and this localized states and V-defect are related to the high optical efficiency. In this work, we investigate the effect of interruption time on the optical and structural properties of high In content InGaN/GaN QW. Especially we studied about the compositional fluctuation of In and V-defect using atomic force microscopy (AFM), photoluminescence (PL), high resolution transmission electron microscopy (HRTEM), and high resolution X-ray diffraction (HRXRD). All samples were grown on c-plane sapphire substrates by metlaorganic chemical vapor deposition (MOCVD). InGaN/GaN QWs with interruption time of 0, 5, 10, 30, 60 sec were deposited after growing the 2 μm thick Si-doped GaN layer at 1130°C. Our AFM measurements revealed that no significant increases of the pit size or number were not observed in the InGaN/GaN. This indicates that interruption time didn't affect on the V-defect formation. In our HRTEM results, The dark contrast in InGaN/GaN QW indicated the QD like or In-rich region. The PL spectra measured at low temperature showed that the luminescence of QD like is much dominant than that of QW. The number and size of

QD like and the thickness of QW are decreased with longer interruption time because of In-re-evaporation during interruption time. As a result, the PL peak positions of QW are blue-shifted and PL peak intensity are decreased as the growth interruption duration becomes longer. This work was supported by Ministry of Science and Technology of Korea and Japan Society for Promotion of Science for joint research between Korea and Japan.

O8.3
HIGH PRESSURE ANNEALING OF GaN FILMS GROWN ON SAPPHIRE. Francis Kelly, Robert Chodelka, Stephen J. Pearton, Mark E. Overberg, Alexander Novikov, Rajiv K. Singh, Reza Abbaschian, Univ. of Florida, Dept. of MS&E, Gainesville, FL.

GaN is an important material due to its unique combination of electronic properties, but processing of GaN is difficult, as is the case with most III-V semiconductors, due to it's tendency towards chemical deterioration at elevated temperatures. Thermal annealing of GaN must therefore be carried out under a high partial pressure of Nitrogen in order to avoid surface degradation from said deterioration. GaN films grown on sapphire (0001) wafers were annealed in a unique high temperature/high pressure system at various temperatures and examined for surface degradation using AFM and SEM. Hall measurements and PL/CL were performed to investigate any concomitant changes in electrical and/or optical properties. Surface roughness changes due to the annealing process are discussed.

O8.4
SURFACE MORPHOLOGY OF GaNAs AND InGaNAs THIN FILMS GROWN BY MBE. M. Adamcyk, B.J. Ruck, J.H. Schmid, S. Tixier, T. Tiedje, University of British Columbia, Department of Physics, Vancouver, CANADA; V. Fink, M. Jeffries, D. Karaiskaj, K.L. Kavanagh, M. Thewalt, Simon Fraser University, Department of Physics, Burnaby, CANADA; Joe Trodahl, Victoria University of Wellington, School of Chemical and Physical Sciences, Wellington, NEW ZEALAND.

Much progress has been made recently on improving the performance of semiconductor lasers that emit in the 1.3-1.55 μm wavelength range, in which the active region consists of the dilute nitride alloy $In_yGa_{1-y}N_xAs_{1-x}$ (x<0.05). In this paper, we report on the evolution of the surface morphology of dilute GaNAs and InGaNAs grown on GaAs by molecular beam epitaxy with atomic nitrogen produced by an RF plasma source. In GaNAs films we find a sharp transition between smooth two dimensional growth and rough three dimensional growth with increasing nitrogen content. Growth conditions which favor high Ga surface diffusion such as high As_2 flux, low growth rate and high growth temperature also favor rough surface formation. Smooth films (2D growth) show the most efficient photoluminescence emission when they are grown at high temperature and high As_2 flux. The transition in the surface morphology for 1% nitrogen occurs at a growth temperature of 520°C, and an As_2/Ga flux ratio of 18. On the three-dimensional-growth side of this transition, in-situ UV light scattering at a wavelength of 250 nm, shows that the surface roughness increases exponentially with time as soon as the GaNAs growth starts, with no critical thickness, unlike dislocation mediated surface roughening mechanisms. Cross sectional scanning electron microscope images show surface slopes consistent with the formation of {111} facets. No evidence of a distinct GaN phase was found in TEM or Raman scattering. Reciprocal space maps made by high resolution x-ray diffraction show that the three dimensional films have a non-uniform N-content. Possible reasons for the morphological transition will be presented, as well as experimental results on the effect of In on the surface morphology transition.

O8.5
STRUCTURE AND LUMINESCENCE OF LOW TEMPERATURE InAs QUANTUM DOTS (QDs) GROWN ON [001] GaAs BY MBE AND SUBJECTED TO THERMAL FLASHING. N.D. Zakharov, P. Werner, Max-Planck-Institute for Microstructure Physics, Halle, GERMANY; D. Bimberg, Technical University, Berlin, GERMANY; G.E. Cirlin, Institute for Analytical Instrumentation RAS, St. Petersburg, RUSSIA; N.A. Maleev, A.R. Kovsh, Henrich-Hertz Institute, Berlin, GERMANY; N.N. Ledentsov, B.V. Volovik, A.E. Zhukov, V.M. Ustinov, Zh.I. Alferov, A.F. Ioffe Physico-Technical Institute RAS, St. Petersburg, RUSSIA.

The growth of InAs QDs arrays on GaAs substrate at relatively low temperature (LT) is motivated by the potential possibility to create long-wavelength laser 1.48-1.55 μm. It was found that the LT QDs may result in photoluminescence (PL) wavelength emission in the range 1.6 - 1.7 μm due to formation of agglomerates of QDs [1]. In our investigations, the InAs QDs were formed on (100) GaAs substrates at 325°C and then covered by GaAs layer of different thickness. At this step, the temperature was increased up to 600°C with the growth interruption at different duration (thermal flash). After this procedure a thick GaAs cap layer was additionally grown. The PL properties of the grown structure depend on the thickness of overgrown GaAs layer and the duration of flashing, which may be attributed to defect reduction [2]. We investigated the samples by PL and different TEM techniques. We found that conglomerates of small InAs QDs formed by InAs 4 ML deposition at 320-350°C usually contain dislocation dipoles. It should be noted that the dislocation core of dipoles always stays in GaAs matrix out of QDs. In some cases the misfit dislocation network was found in the non-flashed specimens. The defect structure formed in the vicinity of InAs QDs depends on thickness of overgrown GaAs layer and flash parameters. The thermal flashing of samples with thin GaAs overgrown layer (about 5 nm) results in almost complete elimination of structural defects (misfit dislocation network, dislocation dipoles) and considerable increase in PL. [1] M.V. Maximov et al., Appl. Phys. Lett. 75, 2347 (1999). [2] N.N. Ledentsov et al., Semicond. Sci. and Technol. 15, 604 (2000).

O8.6
MBE GROWTH MODELING OF InAs(001) ON THE BASIS OF *AB INITIO* DFT, STM AND RHEED. Frank Grosse[a,b], Mark Gyure[b], William Barvosa-Carter[b], Christian Ratsch[a], Richard Ross[b], James Owen[a,b], Jenna Zinck[b]; [a]UC Los Angeles; [b]HRL Laboratories.

Growth simulations of III/V semiconductors can give significant inside into basic physical mechanisms and provide improved growth methods leading to higher quality in device applications. Due to their complex reconstructions, simulating III-V semiconductor growth on relevant length and time scales is a challenging task and makes approximations necessary. On the other hand, to be predictive and to span a wide range of validity, high accuracy in the description of the relevant processes is crucial. We combine theory and experiment, in particular *ab initio* density functional theory with scanning tunneling microscopy and reflection high energy electron diffraction experiments to build a high resolution kinetic Monte Carlo growth model of InAs(001) homoepitaxy valid for growth on singular and vicinal surfaces under a large variety of growth rates (In flux rate) under different As pressures and temperatures. Thermodynamical equilibrium properties including phase transitions between different reconstructions are given within the growth model solely by *ab initio* calculations, the remaining parameters describing the growth kinetics, namely the In transition energy and prefactors, are determined by comparison to desorption experiments and island size distribution. With our model we are able to explain non-intuitive trends with increase of As pressure, i.e. closer to step flow on vicinal surfaces and larger islands in the low coverage regime, in excellent agreement with STM observations.

O8.7
EVOLUTION OF COHERENT InAs QUANTUM DOTS ABOVE THE COHERENT CRITICAL THICKNESS WINDOW BY METALORGANIC CHEMICAL VAPOR DEPOSITION. T.S. Yeoh and J.J. Coleman, Semiconductor Laser Laboratory, Urbana, IL; C.P. Liu, National Cheng Kung University Tainan, TAIWAN; Y. Kim, Materials Research Laboratory, Urbana, IL.

The evolution of Stranski Krastanow grown InAs quantum dots on GaAs was examined by varying the deposition thickness and growth interruption times. We have grown coherent InAs quantum dot layers with depositions within and above the theoretical monolayer coverage window for the generation of defect-free quantum dots by atmospheric pressure metalorganic chemical vapor deposition. As with other metalorganic chemical vapor deposition systems, a low V/III ratio during growth is critical to the formation of fully coherent islands. The resulting dots of densities exceeding $4.9x10^{10}$ cm^{-2} were found to have a lower critical thickness of formation and a smaller diameter than previously reported. By correlating photoluminescence and transmission electron microscopy of quantum dots capped at various growth interruption intervals, we found the growth interruption time to be a critical factor in generating defect-free quantum dot ensembles for coverages exceeding the critical thickness. Densities exceeding $1X10^{11}$ cm^{-2} for coherent dots were found for samples at and above the theoretical critical thickness for APMOCVD and MOCVD for specific time windows with no change in incoherent dot densities. Our results imply that the incoherent dots are generated only after the coherent dot density reaches a maximum density whereupon any remaining source material from the wetting layer becomes incorporated into dislocated quantum dots. This nucleation rate difference between coherent and incoherent dot formation allows us to engineer unique, metastable quantum dot structures at and above the window for defect-free quantum dots.

O8.8
GROWTH OF COMPOUND SEMICONDUCTORS IN NANOMETER SIZED CHANNELS OF POLYMERS. R. Engelhardt and R. Koenenkamp, Hahn-Meitner Institut, Berlin, GERMANY.

Using solution growth techniques we have prepared compound semiconductors as vertical columns in nanometer diameter channels in

polymer foils. The polymer foils are first exposed to irradiation by heavy swift ions, then exposed to an appropriate etch solution. The ion irradiation leads to the formation of narrow ion tracks of nearly amorphous structure. Upon exposure to the etch solution these regions etch preferentially. Vertical channels of well defined geometry with diameters as small as 30 nm are formed in the etching process. We demonstrate the controlled growth of polycrystalline semiconductors in these channels. Upon removal of the polymer vertically aligned semiconductor columns with large aspect ratios and nanometer diameters remain. Device applications will be discussed.

O8.9
STRUCTURAL EVOLUTION OF PSUDOMORPHIC InSb MOLECULAR LAYER ON Si(001) AND Si(111) SUBSTRATES. B.V. Rao, D. Gruznev, T. Tambo, C. Tatsuyama, Toyama University, Toyama, JAPAN.

Growth of InSb on Si substrates is very difficult due to the presence of over 19% lattice mismatch. This mismatch is much larger than the theoretically predicted 12-14% mismatch for the psudomorphic growth. This large mismatch results in the formation of 3D islands much before the completion of first InSb molecular layer. Recent results of InSb growth on GaAs showed that at a nominal coverage of about 90ML InSb covers whole of the GaAs surface ($\approx$15% mismatch). In and Sb are well-known surfactants in the Si industry, which are known to modify the growth kinetics on Si surface. Present study illustrates how the In-induced surface reconstructions of Si substrates can be used to achieve psudomorphic growth of InSb on Si. Sb adsorption on Si(001)-In(4×3) reconstruction at 280°C results in the formation of a 2×8 ordered psudomorphic InSb molecular layer, where the large unitcell of 4×3 reconstruction acts as a nucleation site. The large strain due to the lattice mismatch seems to have relieved by the formation of periodic defect structures. This 2×8 structure can be compared to the InSb(001)2×8 reconstruction. On the other hand, Sb adsorption on Si(111)-In(4×1) completely replaces the Si-In bonds by Si-Sb bonds. This replacement seems to soften the poorly reactive Si-Sb interface with the formation of well ordered Si(111)-Sb(2×1) reconstruction at 300°C (Sb deposition on Si(111)7×7 surface below 550°C produces only disordered phase). The replaced In atoms reorder on this 2×1 phase to form a psudomorphic InSb molecular layer with 2×2 structure. Again, this structure is comparable to the InSb(111)2×2 reconstruction. We detail the difference in the structural evolution of Si(001)-InSb(001)B and Si(111)-InSb(111)A molecular layers.

O8.10
INFLUENCE OF TEMPERATURE AND ION KINETIC ENERGY ON SURFACE ROUGHNESS OF THIN FILMS FABRICATED BY DUAL PLASMA DEPOSITION. L.P. Wang, K.Y. Yu, X.B. Tian, B.Y. Tang, and P.K. Chu, City Univ of Hong Kong, Kowloon, HONG KONG.

The surface roughness of thin films affects the crystalline properties as well as their applications and is preferably as small as possible. In our experiments on the fabrication of CeO_2 thin films on Si(100) substrate by dual plasma deposition, we investigate the influence of the substrate temperature and ion kinetic energy on the surface roughness. The roughness decrease with increasing substrate temperature, possibly due to enhanced diffusion of the adatoms. A higher ion bombardment energy has a similar effect and it is also believed to be related to the surface diffusion of adatoms. We have also found that when a DC voltage is applied to the substrate and the film is thick to withstand electrical breakdown, the surface is rougher. On the other hand, when the film is thin and the applied DC voltage can cause breakdown in the film, the film exhibits smaller results. We will present our experimental results as well as a mechanism to explain the data.

O8.11
MICROSTRUCTURE OF ORGANIC THIN FILMS OF ELECTROLUMINESCENT MOLECULES STUDIED BY GRAZING-INCIDENCE X-RAY DIFFRACTION. Detlef-M. Smilgies, CHESS, Cornell Univ, Ithaca, NY; Ed Kintzel Jr., James G. Skofronick, Florida State Univ, Physics Dept, Tallahassee, FL; Hisao Yanagi, Kobe University, Dept of Electrical Engineering, Kobe, JAPAN.

Recently thin films of small aromatic molecules have received a lot of attention for their potential use in light-emitting diodes and organic transistors. The advantage of small molecules over the commonly used light-emitting polymers is, that they can be grown in crystalline form and their electronic and optical properties can thus be better understood and controlled. Single-crystalline films have been found to have narrower optical emission spectra and to emit polarized light. Furthermore it is hoped that single crystalline films can be grown with smaller defect densities than polycrystalline films and thus have a longer lifetime in devices. An important step in the development of crystal growth techniques is the characterization of the microstructure of such films. We have employed synchrotron-based grazing-incidence x-ray diffraction (GIXRD) to study films of p-quaterphenyl (p-4P) and POPOP which were grown by molecular beam epitaxy on alkali halide surfaces. GIXRD allows to identify various crystalline phase growing simultaneously, different orientations of the surfaces of the crystallites, as well as epitaxial alignments of the crystallites with respect to the substrate, even in very complex systems. Furthermore, the domain structure of the film can be characterized, which is a dependent on both the substrate symmetry as well as the symmetry of the crystallites forming the films. Applications will be illustrated by recent results on thin films of p-4P on NaCl(001) and POPOP on KCl(001).

O8.12
STUDY OF DIFFERENT PHASES IN a-C:H:N THIN FILM DEPOSITED BY PLASMA-ENHANCED CHEMICAL VAPOUR DEPOSITION: A COMPARISON BETWEEN THEORETICAL AND EXPERIMENTAL DATA. F. Antoniella, L. Valentini, Materials Engineering Center, Perugia Univ, Perugia, ITALY; A. Continenza, L. Lozzi, S. Santucci, L'Aquila Univ, Dept of Physics, L'Aquila, ITALY.

The growth of nitrogen doped amorphous carbon compounds (a-C:H:N) thin films is an important issue in the material science because of their interesting properties, such as high hardness, low friction coefficients, chemical inertness. These films are generally prepared by means of Ar^+ plasma assisted chemical vapour deposition. During the growth of these materials an important effect is the formation of different phases because of the use of high energy ions. The aim of this work is to study the growth of (a-C:H:N) films deposited with plasma decomposition of CH_4/N_2 and $CH_4/N_2/Ar$ mixtures, with different methane and nitrogen fluxes. In order to understand the stoichiometry and give some insights on the possible phases present in the compounds, we compared the X-ray and Soft X-ray photoemission valence band spectra with an ab–initio study using the full–potential linearized augmented plane wave (FLAPW) method[1] on some selected ordered C-N phases such as C_3N_4, CN, diamond and graphite).
[1]H.J.F. Jansen and A.J. Freeman, Phys. Rev. B **30**, 561 (1984).

O8.13
APPARATUS DEVELOPMENT FOR DIAMOND SYNTHESIS FROM ACETONE VAPOR WITH LOW ENERGY CONSUMPTION. Fumitomo Onishi, Rie Hayashi, Yoshiki Takagi, Division of Materials, Teikyo Univ. of Science & Technology, Yamanashi-pref., JAPAN.

We synthesized diamond via gaseous phase of vaporized acetone. Molecular acetone decomposes to two methyl radicals with activation. We propose here a new method for diamond synthesis with these methyl radicals from molecular acetone. With this method, we successfully synthesized diamond particles with shorter experimental time. With liquid carbon source, such as acetone, substitutional impurity elements will be easily controlled in synthesized diamond thin film for the future electronic device applications.

O8.14
DIAMOND SYNTHESIS ON OXIDE SUBSTRATES. Rie Hayashi, Fumitomo Onishi, Yoshiki Takagi, Division of Materials, Teikyo Univ. of Science & Technology, Yamanashi-pref., JAPAN.

Recently, many results were reported by many institutes and companies all over the world for diamond particles or thin films synthesized on crystalline substrates, such as molybdenum, silicon etc. But diamond on oxide or amorphous substrates, were rarely reported. In this study, we used oxide materials as substrates, for example, quartz glass, borosilicate glass (PYREX), alumina, etc. We used unique apparatus of diamond synthesis. It is on our completely closed system, no reaction gas was introduced to the chamber and no reactant gas was evacuated from it. Graphite rod was used as carbon source, mounted the center the chamber, about 3-4mm under the rod, the oxide substrates were set. Hydrogen gas was introduced into the reaction chamber with the suitable initial pressure, and then sealed. Graphite rod was heated and controlled with Joule heating. The typical reaction time was 40 min. With SEM photographs, crystal shaped particles were observed. And with Raman spectrometry, Raman peaks were assigned as typical diamond peaks. The results have been duplicated. With these results, we clearly confirmed that the deposits on oxide substrates were diamond particles. And We compared results of with this unique closed system and conventional flow system.

O8.15
SYNTHESES OF DIBLOCK/SILICA FILMS WITH REGULAR AND REVERSE MESOSTRUCTURES OF LARGE CHARACTERISTIC LENGTH SCALES BY SOLVENT EVAPORATION-INDUCED SELF-ASSEMBLY OF POLYSTYRENE-BLOCK-POLY(ETHYLENE

OXIDE). Kui Yu, C. Jeffrey Brinker, Alan J. Hurd, Sandia National Laboratories, Albuquerque, NM; Thomas P. Rieker, Univ. of New Mexico, Center for Micro-Engineered Materials, Albuquerque, NM; Adi Eisenberg, McGill Univ., Dept. of Chem., Montreal, CANADA.

Mesostructured silica films with large characteristic length scales were synthesized through an evaporation-induced self-assembly procedure, employing amphiphilic polystyrene-block-poly(ethylene oxide) (PS-b-PEO) diblock copolymers as structure-directing agents. The synthesis process begins with a dilute homogeneous solution of a silica precursor and the diblock copolymer in a mixture of tetrahydrofuran (THF) and water. During film formation, THF preferentially evaporates; accordingly, the species in the depositing film increasingly concentrate and the solvent quality for the diblock progressively decreases. At some critical point, cooperative self-assembly of both the PS-b-PEO diblock and the silicate starts. Subsequently, liquid-crystalline mesophases is obtained. From one identical copolymer sample, diblock/silica films with different mesostructures can be synthesized; as the volume ratio of the diblock to silica increases, morphologies of the mesostructures change progressively from regular, through lamellar, to inverted. For the diblock/silica films with regular mesophases, copolymer removal produces mesoposity; the pore size is controlled by the molecular weight of the diblock (at a constant volume ratio of the diblock to silica). The present system is believed to be the first to yield amphiphile/silica films with regular and reverse mesophases, as well as multi-bilayer vesicular mesostructures, through solvent evaporation-induced self-assembly (EISA). The present process of self-assembly goes from dilute to concentrated solution regimes; a comparison of the present system with self-assembly of diblock copolymers in dilute solution and in bulk is presented. A range of similarities of the three systems, such as morphogenic effects of effective volume ratios of the two blocks, is highlighted. Furthermore, the ready formation of the diblock/silica films with multi-bilayer vesicular mesostructures is discussed.

O8.16
AFM STUDIES OF CARBOSILANE DENDRIMER CHEMISORBED ON MICA AND SILICON SURFACE. Zhongdang Xiao, Xiaobin Deng, Aurelie Mayeux and Chengzhi Cai University of Houston, Dept of Chemistry, Houston, TX.

The absorption and binding of $SiCl_3$ or ethenyl groups carbosilane dendrimer on mica and silicon substrates have been investigated by atomic force microscopy (AFM). Multilayer, monolayer and monodispersion images of dendrimer molecules have been obtained on mica surface by AFM. From AFM images, it was observed that the shape of the individual dendrimer was nearly spherical disk and the apparent size was about 20 nm in diameter that convolutes the shape of tip. The binding of dendrimer onto oxidized silicon surface was very strong, which is due to "multipoints binding" of dendrimer that results from the formation of a large number of Si-O bonds at the interface, and annealing could significantly promote such binding. The contact angle of dendrimer monolayer is up to 94°, indicating the preferential adsorption of the end groups on mica and oxidized silicon surface thus exposing a hydrocarbon core to the surface.

O8.17
THE IMPROVEMENT OF THIN POLYMER FILM PROPERTIES THROUGH PLASMA IMMERSION ION IMPLANTATION AND DEPOSITION TECHNIQUE. Elidiane C. Rangel, Nilson C. Cruz, Rogério P. Mota, Roberto Y. Honda, Mauricio A. Algatti, UNESP, Dept of Physics and Chemistry, Guaratinguetá, SP, BRAZIL.

Plasma Immersion Ion Implantation and Deposition (PIIID) is a powerful technique that enables ion bombardment during the deposition process, rendering unique characteristics to the plasma deposited film. Simultaneously to the plasma stablishment, high voltage negative pulses are supplied to the substrate holder. During the off-time of the pulses, species from the plasma are deposited onto substrates as in conventional PECV processes. In the on-time of the pulses, ions from the plasma are accelerated to the biased electrode and implanted in the samples, providing in situ modifications. This work describes the influence of the pulse frequency, ν, on the chemical, optical and mechanical properties of polymer films deposited/bombarded by plasma. The glow discharges employed in this study were excited by radiofrequency power (13.56 MHz, 60W) in acetylene and argon gas mixtures. Negative pulses (25 kV) were supplied to the substrate holder at different frequencies. Infrared and ultraviolet-visible spectroscopy were respectively employed to investigate the chemical structure and the optical constants of the films. Polymer wettability was determined through contact angle measurements using DI water. The resistance of the material to oxidation was studied by its etching rate in oxygen plasmas. Hardness measurements were performed using the nanoindentation technique. It was observed that the film deposition rate increases with increasing ν up to a critical value, decreasing after that. The molecular structure and the chemical composition were also modified in the bombarded samples. Increasing the pulse frequency resulted in an improvement in the resistance of the films to oxidation and in their hardnesses. Film wettability was also sensitive to the pulse frequency, rendering a higher wettability character to the polymer surface. Interpretation of the results is proposed in terms of the ion energy loss mechanisms.

O8.18
CHARACTERIZATION OF CHEMICAL AND SENSORIC PROPERTIES OF ION-BEAM MODIFIED POLYETHERSULFONE LAYERS. Karin Sahre, Klaus-Jochen Eichhorn, Frank Simon, Institute of Polymer Research, Dresden, GERMANY; Margaritha Guenther, Gunnar Suchaneck, Gerald Gerlach, Dresden University of Technology, Institute for Solid State Electronics, Dresden, GERMANY.

Thin chemically modified polyethersulfone films (PES) are increasingly important for application as functional layers for new microelectronic sensors. To modify such polymeric structures the ion implantation is a preferred method as we had shown on aromatic polyimides recently. First, in this paper the detailed studies in the characterization of boron ion-induced molecular modifications of aromatic polyethersulfone layers using methods of vibrational spectroscopy (ATR-FTIR, Raman spectroscopy), X-ray photoelectron spectroscopy (XPS) and spectroscopic ellipsometry are presented. The combination of these analytical methods gives a complete picture of the main processes in the layers. Thus the results of vibrational and X-ray photoelectron spectroscopy indicate that in dependence on dose and energy of implanted boron ions the sulfone bonds are destroyed and carbon-rich, amorphous and graphite-like structures are formed. The shrinking behavior of PES films (10% decrease) and the increase of the refractive index of polymer layers from about 1.6 to 2.0 caused by the implantation at high energy and dose (180 keV, 10^{15}-10^{16} B^+/cm^2) were studied using spectroscopic ellipsometry. To fit the ellipsometric data we used a suitable optical model which represents the physical reality of the samples satisfactorily. Second, sensoric properties of PES films especially the swelling behavior in dependence on relative humidity were investigated using a corresponding bimorphic humidity sensor. The influence of ion-beam induced modification on moisture uptake was determined by Freundlich's coefficient. Results concerning the stress-strain-relationships and the change of the electrical properties dependent on dose and energy of implanted ions are also presented.

O8.19
STRUCTURE MODULATION AND STRAIN RELAXATION MECHANISMS IN FERROELECTRIC THIN FILM. Laurent Lahoche, Lab. Roberval UMR UTC-CNRS, I.U.T. of Amiens, FRANCE; Vladimir Lorman, LPM, CNRS, Univ. of Montpellier 2, Faculty of Physics, FRANCE; Sergei Rochal, Univ. of Rostov on Don, Faculty of Physics, RUSSIA; Jean-Marc Roelandt, Lab. Roberval UMR UTC-CNRS, Univ. of Tech. of Compiégne, FRANCE.

This study investigates the possible stress relaxation mechanisms in ($PbTiO_3$) epitaxial ferroelectric ultra-thin film deposited on (MgO) single-crystalline thick substrate. The main attention is paid to the dielectic, thermodynamical and mechanical properties of the nano-material. The proposed analysis takes into account the inhomogeneous film-substrate coupling together with the specific 2D mechanical boundary condition and the total strain relaxation due to misfit dislocations. For that goal, we develop a phenomenological model which includes a detailed crystallographic analysis of the interface morphology and following thermodynamic consideration. The model is based on the experimental data which reveal a concidence lattice in the interface. It allows us to determine the transformational properties of an induced inhomogenous modulation arising in the film due to its coupling with the substrate. The modulation is then related to one of the irreducible representations of the space group Gf of the ferroelectric material which composes the nano-film. It permits to describe the thermo-electro-mechanical problem in terms of the Gibbs energy density using the coupling between internal variables, namely the order parameter of the superstructure, stress tensor and electrical polarization vector. In order to obtain the stability regions in the thickness-temperature plane and corresponding film nano-structures for different ferroelectric states formed during the deposing process and the successive return to room temperature, we perform the energy minimization. The resulting phase diagram shows different regimes of film growth : i) in the ultra-thin films the surstructure formation mechanism favors the phase with non-trivial unit cell multiplication and the polarization direction perpendicular to the substrate, ii) for the films with the thickness higher than 100 nm 2D-clamping stabilizes usual c-domains and iii) for the intermediate thicknesses, several a-type states can become stable. A numerical modeling of the residual strain level in the film is also proposed for three qualitatively different thicknesses.

O8.20
EFFECTS OF ROUGHNESS OF SUBSTRATES AND OXYGEN

CONTENT ON C-AXIS PREFERRED ORIENTATION OF ZnO FILMS DEPOSITED BY RF MAGNETRON SPUTTERING. Jae Bin Lee, Hyeong Joon Kim, School of MS&E, Seoul National University, Seoul, KOREA.

The c-axis preferred orientation of the piezoelectric film is the most important factor in manufacturing of film acoustic wave devices. The effects of roughness of substrates and oxygen content were investigated on c-axis preferred orientation of ZnO films deposited by radio frequency (rf) magnetron sputtering. The total sputtering pressure was 10mTorr and the oxygen content were varied from 0 % to 70 %. The rms roughness of the used substrates were 1.27, 17.1, 21.1, and 65~118 Å. The crystalline structure and the angular spread of (00*2) plane normal to the as-deposited ZnO films were determined by x-ray diffraction and x-ray rocking curve analyses. The crystallinity and the c-axis preferred orientation of ZnO films strongly depended on not the oxygen contents but the surface roughness of the used substrates. The deposited ZnO films had better crystallinity and higher c-axis preferred orientation on the smoother surface substrate.

O8.21
UNIFORMITY OF C-AXIS ZnO ON A LITHOGRAPHICALLY PATTERNED METAL/DIAMOND SUBSTRATE. Anthony S. Holland, Geoffrey K. Reeves, School of Computer Systems and Electrical Engineering, RMIT University, Melbourne, AUSTRALIA; Patrick W. Leech, CSIRO CMST, Clayton, Victoria, AUSTRALIA.

We report in this paper, on the influence of the topography of a lithographically patterned metal/diamond substrate on the uniformity of sputtered c-axis (002) ZnO films. The substrate consisted of aluminium fingers deposited on a CVD diamond film. (This structure, with c-axis aligned ZnO, is of considerable interest for the fabrication of GHz SAW devices). Diamond films with an average surface roughness of ~1nm, had aluminium fingers (thickness 80nm, linewidth/space 2.6micron) patterned on them. ZnO (thickness 0.5micron) was RF sputtered on to the substrate and the uniformity of the ZnO grain structure was examined using SEM, XRD and AFM. Abrupt changes in the substrate topography at the edges of the aluminium fingers resulted in poor alignment of ZnO grains. SEM/AFM micrographs clearly show the misalignment of ZnO grains at the edges of the raised fingers. XRD has shown both (002) and (101) orientations. These results were compared to a second series of samples where the aluminium fingers (thickness 80nm, linewidth/space 2.6micron) were recessed into the diamond film, using a damascene-like process. Using a photoresist pattern, trenches were ion beam etched in the diamond (depth ~100nm). Aluminium was deposited by RF magnetron sputtering and the samples lapped to remove unwanted aluminium and planarise the metal/diamond surface. SEM/AFM micrographs of these samples showed improved grain uniformity of ZnO and XRD showed a significant increase in the desired c-axis (002) peak. The undesired (101) orientation was now absent. AFM micrographs also showed the improvement in the ZnO surface topography. The surface was more uniform compared with the step features of the ZnO on raised aluminium fingers. The ZnO growth rate was identical for the diamond and aluminium surfaces. We believe this is the first time recessing SAW fingers has been applied to diamond films, prior to ZnO deposition, and the improved quality and c-axis uniformity of the ZnO film should be beneficial in improving ZnO/diamond SAW performance.

O8.22
LOW TEMPERATURE DEPOSITION OF ZnO THIN FILMS ON POLYMER SURFACES BY PLASMA CVD. Hidetaka Anma, Yuuji Yoshimoto, Mariko Tanaka, Koito Manufacturing Co., Ltd. Shimizu, JAPAN; Yoshinori Hatanaka, Research Institute of Electronics, Shizuoka University, Hamamatu, JAPAN.

To reduce the vehicle weight and to protect the environmental pollution recycle thermoplastics resins are increasingly applied to automobile parts. However, these resins have weakness for the degradation against UV light such as discoloration deformation surface roughness and so on . To solve these problems, we attempted to deposit ZnO thin films on a polycarbonate resin (PC) at room temperature by a cathode deposition in the RF CVD method. ZnO thin films coated on a plastic material are investigated on the protection against solar ultraviolet radiation. Generally, ZnO thin films are produced by means of the RF sputtering thermal CVD or Sol-gel methods. All these methods, however, require the higher substrate temperature above 500°C for film coating. These methods cannot be applied to polycarbonate resins coating. We therefore examined the possibility of deposited ZnO thin films at room temperature by the plasma CVD. We used DEZ, Diethylzinc ($Zn(C_2H_5)_2$) as the experimental organic material. It is found that the deposition rate are intensively influenced on the substrate temperature and Rf power. The deposition rate declined with as the substrate temperature increased, the rate rose with an increase in RF power up to 100W, however, the RF power above 100W the deposition rate dropped with as the RF power increased. Further, the ZnO-coated PC plates exhibited remarkably to improve weatherability in a xenon arc test. Microscopic roughness arose by ultraviolet degradation on the uncoated PC surface. On the other hand, the ZnO-coated PC surface exhibited a smooth surface with no cracks after UV light irradiated for 1000 hours. Moreover, SiO_2 /ZnO two films coated PC plates have a hard surface characteristics, therefore, these films are expected hard coating films for the automotive parts.

O8.23
PREPARATION ZnO THIN FILMS BY FACING TARGETS SPUTTERING SYSTEM. M.J. Keum, J.S. Yang, H.Y. Seong, K.H. Kim, Kyungwon Univ, School of Electrical & Electronic Engineering, Kyunggi-do, KOREA; I.H. Son, Shinsung College, Dept of Electrical Engineering, Chungnam, KOREA; S. Nakagawa, Tokyo Institute of Technology, Dept of Physical Electronics, Tokyo, JAPAN.

ZnO thin films were prepared in pure O_2 gas on glass substrate by Facing Targets Sputtering(FTS) apparatus which can control sputtering parameters in wide range. It is important for changing the energy of sputtered atoms because of the crystallographic characteristics of ZnO thin film changed with sputtering parameters. In order to change the energy of sputtered atoms, we controlled the discharge(0.1-0.8A) and the O_2 gas pressure(0.5-2mTorr). Also, the influence of substrate temperature(R.T-300°C), discharge current and film thickness on the properties of the films has been investigated. The c-axis orientation($\Delta\theta_{50}$) was 3.9° at substrate temperature 300°C, discharge current 0.4A, working gas pressure 1mTorr, and film thickness 0.5μm. When the film thicness is over 1μm, c-axis orientation($\Delta\theta_{50}$) of ZnO thin film showed good with increasing working gas pressure or decreasing discharge current. The c-axis orientation($\Delta\theta_{50}$) of ZnO thin film was 3.3° at substrate temperature 200°C, discharge current 0.3A, working pressure 1mTorr and film thickness 3.5μm.

O8.24
REMOTE PLASMA ENHANCED CHEMICAL VAPOR DEPOSITION OF TiO_X FILMS FROM TITANIUM TETRAISOPROPOXIDE. Masatoshi Nakamura, Shinichi Kato, Toru Aoki and Yoshinori Hatanaka, Graduate School of Electronic Science and Technology, Research Institute of Electronics, Shizuoka University, Shizuoka, JAPAN; Dariusz Korzec, Electrical and Electronic Engineering Department, Faculty of Engineering, Shizuoka University, Shizuoka, JAPAN.

TiO_2 films have intensively been investigated as photo-catalytic and hydrophilic materials under UV light irradiation and applied as anti-fog mirror for automobile. Especially, it is known that anatase type crystalline films show good properties for this purpose. In this study, TiO_X films were prepared by remote plasma enhanced chemical vapor deposition (CVD) technique using titanium tetraisopropoxide (TTIP, $Ti(OC_3H_7)_4$). TTIP is preferable because it incorporates no corrosive component in contrast with the compounds of halogen such as chlorides or bromides. In the process including high density ion of $10^{10}/cm^3$, deposition rate was strongly depended by substrate temperature. Negative value of estimated activation energy in this process meant that adsorption and desorption reactions were dominant for surface reaction. Less influence of rf power on deposition rate suggested that energetic species existed enough to dissociate TTIP molecules in gas phase and TTIP transport rate limited deposition rate in this regime. Deposition rate increased up to 50nm/min as TTIP transport rate was increased. The films deposited at low substrate temperature of less than 200°C were amorphous in x-ray diffraction spectra. From FT-IR spectra it was revealed that these films included a large amount of OH groups. In spite of their amorphous state, these films were sensitive to UV light irradiation and showed highly hydrophilic properties. It is suggested that remote plasma enhanced chemical vapor deposition of TiO_X films is effective for the preparation of hydrophilic surface on plastic substrate. Deposition mechanism and good hydrophilicity of the amorphous TiO_X film will be discussed in the presentation.

O8.25
TITANIUM MONOXIDE FILMS ON Cu AND Cu OXIDE: GROWTH MODE OF ROOM-TEMPERATURE DEPOSITED FILMS ON Cu AND EFFECT OF Cu OXIDE. V.M. Fuenzalida, C.R. Grahmann, C. Herrera, R.A. Zarate, Univ de Chile, FCFM, Centro Investigacion Avanzada en Ciencias de los Materiales and Dept Física, Santiago, CHILE; C. Avila, M.E. Pilleux, Univ de Chile, FCFM, IDIEM, Santiago, CHILE.

Polycrystalline copper films >100 nm thick were evaporated on silicon wafers under ultrahigh vacuum conditions leading to an rms roughness of the films ~2 nm. Some of these substrates were oxidized in air to obtain a native copper oxide. TiO films were subsequently deposited onto the "clean" and oxidized copper films from a resistively heated tungsten boat, in situ, at room temperature. The

films exhibited good adherence and were amorphous. XPS also revealed that the TiO films were contamination-free and that the TiO reduced the thin native oxide of the copper substrate from Cu(II) into Cu(I) or Cu(0) and transformed the TiO into TiO_2 at the interface. No reaction between the copper and the TiO was detected. The low-energy ion scattering spectra (LEIS) of the TiO films up to several monolayers of equivalent thickness indicated the presence of copper, thus implying that the TiO grows by the nucleation of islands even at room temperature. Complete coating of the copper film, as revealed by LEIS, was assured only for TiO deposits above 5 nm.

O8.26
ELECTROCHEMICAL PROPERTIES OF SnO_2 THIN FILMS DOPED WITH Bi AND Si FOR NEGATIVE ELECTRODE OF MICROBATTERY. Young-Il Kim, Hee-Soo Moon, Kwang-Sun Ji, Hanyang Univ, Div.of Materials Science and Engineering, Seoul, KOREA; You-Kee Lee, Uiduk Univ, Dep. of Semiconductor Engineering, Kyoungju, KOREA; Jong-Wan Park, Hanyang Univ, Div. of Materials Science and Engineering, Seoul, KOREA.

Tin oxide has been proposed as a promising alternative anode material for microbatteries. It has been reported that its theoretical volumetric capacity is four times larger than that of carbon-based material, while its gravimetric capacity is twice as large. In this experiment, an optimal amount of Si dopant added to SnO_2 film was determined. Then, Bi was added to Si doped SnO_2 films which were prepared with e-beam evaporation to improve both the cycle performance and the reversible capacity. The effects of Si and Bi addition to the SnO_2 films on the microstructure of the thin films deposited on the Mo/Si substrates were investigated. The films with addition of Si only exhibited reductions in aggregation of tin particles and formation micro-cracks, especially at 5mol% Si. However, there still remained cracks, which induce capacity loss during cycling. To improve capacity retention, Bi was added with Si to SnO_2 films, which exhibited the highest reversible capacity of 200 μ Ah/cm^2 - μm at 200th cycle. The films doped with Bi and Si were found to be ill-defined and featureless without noticeable particle aggregation and cracks. However, the films, which underwent cycling tests showed again aggregated tin particles and re-appearing cracks, which induce cell failure during cycling. We believe that some types of Li-Bi phases as mixed-conductor matrices have improved the cycle life.

O8.27
LUMINOUS EFFICIENCY OF AC PLASMA DISPLAY PANELS WITH MgO-TiO_2 PROTECTIVE LAYERS. Younghyun Kim, Rakhwan Kim, Yonguk Lee, Sung Hoon Chung, Jong-Wan Park, Hanyang University, Div. of Material Science and Engineering, Seoul, KOREA.

Development of the protective layers with higher secondary electron emission yield than that of the conventional MgO is necessary to attain both lower driving voltage and higher luminous efficiency in AC plasma display panels. TiO_2 was added to the pure MgO in order to improve the electrical characteristics of AC Plasma Display Panel using electron beam evaporation. As the [TiO_2/(MgO TiO_2)] ratio in the starting materials increased, the cation ratio of [Ti/(Ti Mg)] and the ratio of metal to oxygen of [(Ti Mg)/O] in the films increased gradually, which might result in the change of energy state. The secondary electron emission yield of MgO-TiO_2 films was found to be larger than that of the conventional MgO protective layer. The luminous efficiency of the panel with MgO-TiO_2 protective layer was also much higher than that of the panel with MgO protective layer probably due to its lower discharging voltage. The increase in the luminous efficiency and the decrease in the driving voltage were in good agreement with the result of secondary electron emission yield as expected.

O8.28
HETEROEPITAXIAL AND POLYCRYSTALLINE INDIUM OXIDE FILMS PREPARED BY OXYGEN ION ASSISTED DEPOSITION. Jun-Sik Cho, Younggun Han, Seon-Ju Kwon, Young-Whoan Beag, Seok-Kuen Koh, Korea Institute of Science and Technology, Thin Film Technology Research Center, Seoul, KOREA.

Heteroepitaxial and polycrystalline growth of undoped indium oxide films was carried out on polished YSZ (001) and glass substrates by oxygen ion assisted deposition. The oxygen ion energy was varied from 60 to 500 eV during indium thermal evaporation. The crystallinity and microstructure of the films were closely related to the oxygen ion energy bombarded on the growing surface. Domain structure and preferential orientation in the [100] direction were obtained in the film deposited at 60 eV. Upon increasing the ion beam energy to 500 eV, the domain structure was changed into the grain structure. Depending on the range of ion beam energy, the main effect of energetic ions on the growing surface of the film may be divided into two categories: the enhancement of adatom mobility and the creation of additional nucleation sites by lattice damage. The dependency of electrical properties of the films on the crystallinity and microstructure will be discussed.

O8.29
YTTRIA STABILIZED ZIRCONIA THIN FILMS PROCESSED BY COMBUSTION CHEMICAL VAPOR DEPOSITION. Zhigang Xu, Qiuming Wei, Jag Sankar, NSF Center For Advanced Materials And Smart Structures, North Carolina A&T State University, Greensboro, NC.

Yttria fully stabilized zirconia (YSZ) is a conductor of oxygen ion. It has been widely used as electrolyte in solid oxide fuel cells. Due to its relatively low ionic conductivity, thin film of YSZ is favored in order to minimize the current path in the electrolyte. Combustion chemical vapor deposition (CCVD) has been used to deposit thin films of diamond, especially many kinds of oxides, such as Al_2O_3, Cr_2O_3, SiO_2, YBCO and YSZ. Among techniques to prepare the YSZ electrolyte thin film for fuel cells, CCVD in the open atmosphere has potential of high deposition rate and low operational cost. We have established a liquid fuel CCVD system. Basically, this system consists of a quaternary HPLC pump, an atomizer, a pilot flame and a substrate cooling/holding supporter. Substrate is placed near or at the end of the aerosol flame. A series of parametric experiments have been conducted. Zirconium 2-ethylhexanoate and yttrium 2-ethylhexanoate dissolved in toluene are used as reagents. Thin films are deposited on Si(100) and MgO(100) substrates. Effects on morphology and microstructure of factors such as concentration of solutions, substrate temperature and position of the substrate in the flame are thoroughly investigated to obtain uniform and dense films. The correlation between the reagent composition and film composition is also studied in order to get cubic phase zirconia at room temperature. Effect of high temperature annealing on the microstructure is also studied. The phases of the films are characterized by X-ray diffraction. The morphologies and microstructures of them are studied with scanning and transmission electron microscopy.

O8.30
FORMATION OF $YCrO_3$ THIN FILMS USING RADIO-FREQUENCY MAGNETRON SPUTTERING METHOD FOR A WIDE RAGNE THERMISTOR APPLICATION. Sang-Hun Kim, Jin Hyeok Kim, Jong-Ha Moon, Chonnam National University, Dept of Inorganic Materials Engineering, Kwangju, SOUTH KOREA; Byung-Teak Lee, Chonnam National University, Dept of Metallurgical Engineering, Kwangju, SOUTH KOREA.

$YCrO_3$ thin films were prepared on thermally oxidized silicon wafers by radio-frequency magnetron sputtering method for their potential use as wide range thermistor materials. Microstructure and crystallinity of thin films, deposited and then post annealed at various temperatures (between 600°C/1h and 800°C/1h), were characterized using transmission electron microscopy and x-ray diffractometer. It was observed that an as-deposited sample has an amorphous phase. Mixtures of an amorphous phase and a crystalline phase were observed in a sample annealed at 600°C/1h, and completely crystallized $YCrO_3$ thin films were observed in samples annealed at above 700°C/1h. Resistance change of a $YCrO_3$ thin film was studied as a function of temperature. A $YCrO_3$ thin film, deposited at 200°C, with a RF power of 100 W, working pressure of 4 mTorr with an Ar/O_2 ratio of 25sccm/25sccm, and then annealed at 800°C/1h, showed a linear characteristic in the log sT vs 1/T plot in the temperature ranges between 300°C and 800°C, showing potential for developing a temperature sensor

O8.31
FORMATION OF A Co_3O_4 TOP LAYER IN SiO_2 COBALT CONTAINING COATINGS SOL-GEL OBTAINED. H. Tototzintle-Huitle, A. Ramos-Mendoza, A. Mendoza-Galván, J. González-Hernández, Centro de Investigación y de Estudios Avanzados del IPN, Unidad Querétaro, MEXICO; B.S. Chao, Energy Conversion Devices, MI.

We have prepared SiO_2 coatings containing cobalt by the sol-gel method on glass substrates. It has been found that in coatings with high Co content, the formation of a Co_3O_4 top layer is promoted under thermal annealing in air. We have studied coatings with a Si to Co nominal atomic ratio of 1.3 with optical, x-ray and Auger depth profile measurements. Thermal annealing were performed by 10 min at temperatures from 300 to 500°C in steps of 50°C. Also, isothermal annealing at 400°C at different times from 10 to 210 min were carried out. From the x-ray diffraction patterns the cubic spinel structure of Co_3O_4 was detectable. The reflection and transmission optical spectra in each, temperature and time annealing series, can be described with an air-Co_3O_4-SiO_2:Co^{2+}-substrate system. From this, the cobalt oxide thickness was obtained as a function of both annealing parameters, temperature and time. For the temperature range studied, it was found an activation energy of 0.41 eV for the cobalt oxide growth, from an Arrhenius plot. The layer thickness follows a

parabolic behavior, which suggests a diffusion-controlled process. The Auger depth profile obtained from a sample annealed at 500°C supports the optical model used.

O8.32
ELECTRODE CHARACTERISTICS OF SPUTTERED LITHIUM MANGANESE OXIDE FILMS WITH DIAMOND-LIKE-CARBON TOP LAYER. Hee-Soo Moon, Kwang-Sun Ji, Hanyang Univ, Div of Materials Science and Engineering, Seoul, KOREA; Won-Il Cho, Young-Soo Yun, Korea Institute of Science and Technology, Seoul, KOREA; Jong-Wan Park, Hanyang Univ, Div of Materials Science and Engineering, Seoul, KOREA.

There have been increasing interests in lithium rechargeable batteries, especially microbatteries, with rapid development of potable electronic equipments and MEMS(Micro electromechanical systems) technology. In this work, lithium manganese oxide, as a strong candidate for the battery materials, which is more abundant, stable in ambient state and less toxic than the other oxides such as lithium nickel oxides and lithium cobalt oxides, was deposited by rf magnetron sputter. The effect of thermal treatment on the microstructure and electrode characteristics of lithium manganese oxide cathode was investigated. In operation of all-solid-state microbatteries, battery failure would be caused by electrode/electrolyte interface reaction, internal stress, degradation of electrode and electrolyte materials during charging/discharging process and so on. In this research we focus on interface reaction problem such as increasing internal resistance which would affect the cyclability and lifetime of microbattery. In order to reduce the interface reaction during operation, we introduce DLC(Diamond-like-Carbon) film that has high electrical resistivity, mechanical hardness and chemical stability. DLC film was deposited on sputtered lithium manganese oxide electrode by ECRCVD(Electron Cyclotron Resonance Chemical Vapor Deposition). Before DLC film was deposited, post thermal treatments were adopted to gain proper crystallization of spinel lithium manganese oxide. The crystal structure of the samples after and before cycle tests was characterized by X-ray diffraction, surface analysis was done by SEM and AFM. The bonding state of lithium manganese oxide was analyzed by XPS and FT-IR. For electrochemical tests, half cells were made with the lithium manganese oxide as cathode, the lithium metal as anode, and 1M solution of $LiPF_6$ in EC-DMC(1:1) as electrolyte. Charge-discharge experiments were performed by cut-off voltage (4.2~3.0V) and current density ($50\mu A/cm^2$). Impedance measurement was used to analyze the internal resistivity of the electrode.

O8.33
HIGH SPATIAL RESOLUTION SOFT X-RAY PHOTOEMISSION STUDY OF WO_3 THIN FILMS. S. Santucci, L. Lozzi, M. Passacantando, INFM and L'Aquila Univ, Dept of Physics, L'Aquila, ITALY; S. La Rosa, N. Yu. Svetchnikov, Sincrotrone Trieste S.p.A., Trieste, ITALY.

Tungsten trioxide (WO_3) is a wide gap n-type semiconductor and it is the subject of an intense both theoretical and experimental studies because of its interesting applications, such as gas sensors towards different gases, like NO_2 and H_2S, and as electrochromic film. Many of these possible applications are mainly due to the oxygen vacancies. For example, in the sensing mechanism, the gas species are adsorbed on the surface changing the concentration of the free electrons on the surface. These electrons are present on the surface because of the oxygen vacancies. The variation of this concentration modifies the electrical conductivity of the film. Similarly, the presence of substoichiometric WO_{3-x} compounds, determines the optical properties of these films. An important parameter in the preparation of WO_3 thin films is the thermal treatment following the sample growth. For example it has been shown that the gas sensitivity and response time are strongly influenced by the annealing procedure, because of the phase transitions induced by the annealing. In this work the WO_3 surface chemical composition has been studied by means of high resolution soft X-ray photoemission spectroscopy. We have studied the surface properties of both as deposited samples and samples after annealing in air at high temperatures. Valence band and W 4f core levels have been analysed on different samples positions and high resolution maps have been acquired. The valence band spectra have shown W 5d density of state at the Fermi level, indicating the presence of metallic tungsten on the surface. This has been confirmed by the W 4f signal, which present both metallic and oxidized phases. The high resolution maps, obtained following both valence and core states, have clearly evidenced the presence non stoichiometric areas and of some metallic islands.

O8.34
IN SITU XPS STUDY OF PHASE AND STRUCTURE-MORPHOLOGICAL CHANGES OF THIN OXIDE FILMS OF GROUP IVA, VA METALS FORMED IN UHV ON Si. N.M. Sushkova, A.G. Akimov, Inst of Physical Chemistry, Russian Academy of Sciences, Moscow, RUSSIA.

Native silicon oxide degrades the quality of IC semiconductor devices made on Si surfaces and its presence is usually hard to avoid. Interactions of group IVA and VA thin metal films with native oxide on Si substrates are of interest since they can reduce the native oxide without damaging the silicon surface structure. These interactions are especially important in formation of epitaxial silicides of group VIII metals, which are used as conducting layers or interconnects in integrated circuit fabrications. Phase formation and change in morphology of Ti, V, Nb and Zr oxide films with thickness up to 2.0nm on Si[100], Si[111] with native oxide layer have been studied by XPS in situ. The metal oxides were formed by the interaction at room temperature in UHV of single- and multi-step deposited of Ti, V, Nb or Zr with native oxide. They passed three fields of phase formation before reached "layer by layer" growth mode. The formation of clean silicon regions during the growth of three-dimensional metal oxide islands was observed. The difference in magnitudes of the metal particle moments, when they hit the native oxide surface, influences the character of metal particle interactions with native oxide. The structure of native silicon oxide surface was crucial for the formation of three-dimensional metal oxide islands.

O8.35
MICROSTRUCTURE OF HETEROEPITAXIALLY GROWN ANATASE AND RUTILE TiO_2 FILMS BY MAGNETRON SPUTTERING. M. Yamagishi and Y. Shigesato, Aoyama Gakuin University, Tokyo, JAPAN.

On account of the strong oxidizing power of the photogenerated holes, the chemical stability and the nontoxicity, titanium dioxide (TiO_2) is the most investigated photocatalyst up to date. Such photocatalytic properties should be heaily affected by the microstructure and surface morphology of the films. In this study $Ti)_2$ films were deposited by r.f. reactive magnetron sputtering on to the following 4 different kinds of substrates, (a) non-alkali glass (Corning #7059), (b) MgO (100), (c) $SrTiO_3$ (100) and (d) rutile (110), (001), (100), where (b)-(d) were single crystals. Deposition conditions were the same for all substates, i.e., 40% O_2 flow ratio [O_2/(Ar+O_2)], total gas pressure of 1 and 3 Pa, substrate temperature (Ts) of 200° and 400° and r.f. power of 200W. X-ray diffraction and pole figure analyses revealed that TiO_2 films on (a) were anatase polycrystals with (101) preferred orientation, whereas hetero- or homoepitaxial growth of anatase or rutile TiO_2 was observed on the (b)-(d) substrates. The epitaxial relationsihps were as follows, (b) anatase (100)[001]/MgO(100)[001], (c) anatase (001)[100] // $SrTiO_3$ (100)[001] and (d) rutile homoepitaxy. It was also found from FE-SEM images that the Ts heavily affected the microstructure and surface morphology of the films, which could be clearly explained in terms of "Thornton's zone model" considering the normalized Ts by the phase transition temperature from anatase to rutile and the melting temperature of rutile.

O8.36
SURFACE TOPOGRAPHY CONTROL OF THE Al AND Al_2O_3 THIN FILMS DEPOSITED BY USING PULSED DC MAGNETRON SPUTTERING. Jinjun Qiu, Kebin Li, Guchang Han, Zaibing Guo and Yihong Wu, Data Storage Institute, National University of Singapore, SINGAPORE.

The thickness of the Al_2O_3 layer used in the magnetic tunneling junctions FM1/Al_2O_3/FM2 is less than 2nm, here FM1 is for the ferromagnetic layer 1 and FM2 is for ferromagnetic layer 2. In order to obtain ultra-thin Al_2O_3 layer with higher breakdown voltage and pin-hole free, extremely smooth surface roughness of this layer is required. Various deposition methods are used for fabrication of this ultra-thin alumina layer. But the Al_2O_3 layer is formed either by oxidation of ultra-thin Al thin film or directly reactively deposition. In this presentation, the surface topography of Al and Al_2O_3 thin films will be extensively studied. The Al and Al_2O_3 thin films were deposited on Si wafer with or without buffer layer (Ta or Ta/NiFe are used as buffer layer) by using DC pulsed magnetron sputtering under ultra-high vacuum system (UHV) at room temperature. The modulation DC pulsed frequency can be adjusted from 2kHz to 20kHz, a RF bias can be applied to the substrate during the deposition, the frequency of the RF source is varied from 300kHz to 600kHz, the Vpp value of the RF bias can be adjusted from 10V to 100V. The Al_2O_3 thin films are fabricated either by using reactively magnetron sputtering or plasma oxidation of Al thin film. The structures of the thin films are characterized by standard x-ray diffraction using the Cu k α line (0.154nm). The surface topography is obtained by atomic force microscopy (AFM) and scanning electron microscopy (SEM). Auger electron spectroscopy is used to examine the chemical composition of the alumina thin films. The as-deposited thin films are usually amorphous, crystalline alumina films can be obtained after the samples are annealed at proper temperatures. Very smooth Al thin film with rms=0.16nm can be sputtered on Si wafer with Ta buffer layer at f=20kHz (DC pulsed frequency) and with RF substrate biasing (V_{pp} is about 21V). The influence of the sputtering

gas, substrate bias, DC pulsed frequency, DC pulsed power, and buffer layer on film growth and properties will be reported in the presentation in more detail.

O8.37
ZINC OXIDE/COPPER OXIDE MIXED FILMS DEPOSITED BY MOCVD. Yuneng Chang, Chihshiang Yeh Lunghwa Inst. of Tech., Dept of Chemical Engineering, Gueishan, Taoyuan, TAIWAN ROC.

Zinc oxide and copper oxide are the basic ingredients for methanol synthesis catalysts. Recent research showed the phase boundary between ZnO domain and Cu2O domain were of great importance to catalyst surface activities. In this research, we used chemical vapor deposition (CVD) technique to prepare ZnO/Cu2O phase intermixed thin films, and identified the growth characteristics. Processing condition studied were as followed: deposition temperature from 360°C to 440°C, partial pressures of oxygen, 190-380 torr, precursor copper acetylacetonate (Cu(acac)2), 0.21 torr, and zinc acetylacetonate(Zn(acac)2), 0.45 torr. AES, and XPS analyses showed average film elemental content being Cu, 52%, Zn, 11%, O, 37%. Copper presented as Cu(I), and Zn as Zn(II). SEM and XRD results indicated that deposited films were of polycrystalline with composite structure. A representative film had a continuous thin ZnO phase bottom layer of flat surface, equiax fine grained; the top of such layer were covered by discrete irregular shaped coarse Cu2O grains. Primary Cu2O phases were (110), (111), and (200). ZnO phases were (002), and (103). SEM showed the impact of deposition temperature on the average Cu2O grain size. Such data were used to estimate the activation energy for grain growth. In fact, to our experiences accumulated in these studies, binary metal oxide CVD showed a wide spectrum of results on film microstructure and morphology. These phenomena reflect a situation caused by both thermodynamics as film composition, and kinetics as transfer/reaction rate, and will be discussed briefly in this paper.

O8.38
WEAK BONDING OF ALUMINA COATINGS ON Ni(111). Emily A.A. Jarvis, Asbjorn Christensen and Emily A. Carter, Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, CA.

We examine the structure and stability of an ultrathin ceramic film coating a metal substrate, specifically, an α-alumina, Al_2O_3, film grown on fcc nickel. This metal-ceramic interface may play a role in materials failure of current combustion engine thermal barrier coatings; the engine is composed of a primarily nickel alloy, and the alumina "coating" layer thickens with repeated thermal cycling due to oxidation of aluminum in the metal alloy. Accordingly, we study the effect of increasing alumina film thickness on the nickel-alumina interface using periodic slab density functional theory within the generalized gradient approximation. Since nickel forms stable alloys with aluminum, it is not obvious whether the bonds between nickel and alumina will be Ni-Al, Ni-O, or both. Interestingly, our calculations indicate that the preferred bonding mode depends on the thickness of the alumina film. Namely, for one monolayer of alumina, the alumina appears amorphous and both Ni-O and Ni-Al interactions take place, while for two and three monolayers, Ni-O interactions decrease and Ni-Al bonds become more pronounced. By studying the effect of increasing alumina thickness on the Ni substrate, we observe a marked decrease in the work of adhesion for thicker alumina coatings. Insight regarding the work of adhesion trend is provided through analysis of the electron density and electron localization function values. Our findings provide a new atomic-scale explanation for the observed increase in spallation with increasing thickness of oxide layer (alumina) that forms during preparation and operational cycling of thermal barrier coatings. The thickest alumina layers energetically prefer intra-ceramic bonding over Ni-Al_2O_3 interface formation. Connections to metal catalyst-oxide support interfaces are also discussed.

O8.39
ELECTRICAL CHARACTERIZATION OF CARBON-DOPED Ta_2O_5 FILMS. K. Chu and J.P. Chang, Department of Chemical Engineering, University of California, Los Angeles, CA; M.L. Steigerwald, R.M. Fleming, R.L. Opila, D.V. Lang and C.D.W. Jones, Bell Labs, Lucent Technologies, Murray Hill, NJ.

Tantalum pentoxide films have the potential to replace SiO_2 in next generation dynamic random access memory (DRAM) fabrication due to its high dielectric constant (k=25). The advantage of low-temperature deposition of Ta_2O_5 (<500°C) also makes it a good candidate for metal-oxide-metal (MOM) capacitors since it is compatible with the aluminum metallization scheme. With pulsed-dc reactive and RF-magnetron sputtering of Ta_2O_5 performed in an argon/oxygen/carbon-dioxide plasma, we have systematically varied the amount of carbon incorporation in the Ta_2O_5 films and investigated its effect on the leakage current of Ta_2O_5 films. In the thick (700 Å) Ta_2O_5 films, an optimal amount (0.8 - 1.4 a.t.%) of carbon doping reduced the leakage current to 10^{-8} A/cm^2 at 3 MV/cm, a four order of magnitude reduction in comparison to a leakage current of 10^{-4} A/cm^2 in a pure Ta_2O_5 film, yet a three order magnitude increase is seen in films with more than 2 a.t.% carbon. Carbon doping, however, shows no improvement in the leakage current in thin (100Å) Ta_2O_5films. Since the same improvement is not seen in thin (100Å) films, it is apparent that the carbon incorporation is not effective in lowering the Fermi level below the defect band. For carbon-doped thick films where the steady state current is negligible, it is likely that the defect band does not span the width of the film. The introduction of an optimal amount of carbon (0.8 - 1.4 a.t.%) reduces the steady state current in positive bias by decreasing the number of defects and interrupting the defect band. X-ray Photoemission Spectroscopy (XPS) data shows the presence of carbonate in these electrically improved carbon-doped films. On the other hand, the photoconductivity results indicate that carbon is terminating electrically active defect sites such as oxygen vacancies in the bulk of Ta_2O_5films.

O8.40
HETEROEPITAXIAL GROWTH AND PHASE TRANSITION PROPERTIES OF VANADIUM DIOXIDE THIN FILMS ON DIFFERENT ORIENTATIONS OF SAPPHIRE SUBSTRATES. Zhaoping Wu, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, CHINA; Hiroshi Naramoto, Japan Atomic Energy Research Institute, Takasaki, Gunma, JAPAN.

Vanadium dioxide (VO_2) thin films deposited on different sapphire substrates have been investigated using XRD, x-ray pole figure, RBS/Channeling and electrical measurements. The results show that VO_2 films grow epitaxially and exhibit strong substrate dependence. Different substrates result in different defect microstructures, i.e., 120° twin (triplet) for VO_2 film grown on (0001) sapphire, 180°(single) twin on $(11\bar{2}0)$ and no twin on $(01\bar{1}2)$ have been observed, which depend on the surface symmetry of the substrate and the mismatch between the sapphire and VO_2 film. Moreover, the films deposited on $(10\bar{1}0)$ sapphire are composed of two mixed monoclinic phases, namely M1 and M2. M1 phase is unstable because of the existence of larger misfit strain in the $(\bar{1}02)$ VO_2 film. The reduction of misfit strain in the film prefers the formation of M2 phase. The x-ray diffraction and pole figure results show that both M1 and M2 phase are well aligned with the substrate and both contain twinned structure. Therefore, the microstructure of the film can be illustrated as transversely modulated heterophase polydomain. Higher electrical resistivity ratio of semiconductor phase to metallic phase can be achieved only in VO_2 thin film with single phase, either M2 or M1 phase. The phase mixing degrades the ratio of resistivity of two phases. The film with single M2 phase exhibits lower transition temperature of 58°C without any degradation of the phase transition properties.

O8.41
CRYSTALLIZATION KINETICS OF AMORPHOUS TiO_xN_y. Kyle Hukari, Rand Dannenberg, AFG Development Corporation, Petaluma, CA; E.A. Stach, Lawrence Berkeley Laboratory.

A series of amorphous TiO_xN_y films are sputter deposited onto amorphous Si3N4 transmission electron microscope grids. The activation energy, transformation velocity pre-exponentials, and nucleation rates are extracted from in-situ heating stage TEM videotape. These variables are substituted into the Johnson-Mehl-Averami equations, and with very minor changes, result in fraction transformed vs. time curves that fit the experimental data very well. The impact of nitrogen incorporation on the kinetics of TiO_xN_y crystallization is discussed.

O8.42
MICROSTRUCTURE AND SURFACE EVOLUTION IN THE CRYSTALLIZATION OF α-Fe_2O_3/α-Al_2O_3(0001) FILMS. Tae Sik Cho, Sangju National Univ, Dept of Materials Science and Engineering, Sangju, KOREA; Seok Joo Doh, Jung Ho Je, POSTECH, Dept of Materials Science and Engineering, Pohang, KOREA; Min Su Yi, Do Young Noh, K-JIST, Dept of Materials Science and Engineering, Kwangju, KOREA.

The microstructure and surface evolution in the crystallization of amorphous α-Fe_2O_3/α-Al_2O_3(0001) films has been studied using real-time synchrotron x-ray scattering and atomic force microscope. We find that a very thin(~50-Å-thick), epitaxial, α-Fe_2O_3 and Fe_3O_4 interfacial islands are formed on α-Al_2O_3(0001) in the as-deposited films. The amorphous precursor is crystallized in three steps to the epitaxial α-Fe_2O_3 grains with annealing temperature. The first step is the growth of the well aligned, preexisting, α-Fe_2O_3 interfacial islands on α-Al_2O_3(0001), and the transformation of the Fe_3O_4 islands to the α-Fe_2O_3 phase. The second step is the regrowth of the misaligned, homoepitaxial, α-Fe_2O_3 grains on the well aligned domains from

400°C, resulting in the increase of surface roughness. Finally the heteroepitaxial misaligned grains start to nucleate directly on the α-Al_2O_3 substrate at the high temperature of 600°C. The evolution of surface roughness is caused by the microstructure evolution during the crystallization of the amorphous precursor films.

SESSION O9: MISCELLANEOUS
Chairs: George H. Gilmer and M. V. Ramana Murty
Friday Morning, April 20, 2001
Salon 7 (Marriott)

8:30 AM O9.1
CALCULATIONS OF SURFACE STRUCTURE FOR $SrTiO_3$ PEROVSKITE. E. Heifets[a,b], R.E. Cohen[a,b], R.I. Eglitis[c], E.A. Kotomin[c,d] and G. Borstel[c], [a]Carnegie Institution of Washington, Washington, DC; [b]Seismological Laboratory, California Institute of Technology, Pasadena, CA; [c]Dept. of Physics, University of Osnabrueck, Osnabrueck, GERMANY; [d]Institute of Solid State Physics, University of Latvia, Riga, LATVIA.

We present and discuss results of the calculations of the surface relaxation for $SrTiO_3$ surfaces with different terminations using a wide variety of methods of computational physics, such as *shell model* as well as *ab initio* methods based on HF and DFT formalism. By means of semi-empirical shell model, the positions of atoms in 16 near-surface layers placed atop a slab of rigid ions are optimized. This permits us determination of a surface rumpling and surface-induced dipole moments (polarization) for different terminations of the (100) and (110) surfaces. Simultaneously, we performed *ab initio* calculations with three top planes allowed to relax. Our shell model results for the (100) surfaces are in good agreement with both our *ab initio* calculations and LEED experiments. For the (110) $SrTiO_3$ surfaces O-termination is predicted to be the lowest in energy.

8:45 AM O9.2
PREPARATION AND CHARACTERIZATION OF (Ba, Sr)TiO_3THIN FILMS BY LIQUID SOURCE CHEMICAL VAPOR DEPOSITION. Young Ki Han, Cheol-Hoon Yang, Dong-Hyun Kim, Geun-Jo Han, Ki-Young Oh, Ju Ho Song, and Chul-Ju Hwang, JuSung Engineering Co., Kyunggi-Do, KOREA; Jaehoo Park, Cheol Seong Hwang, Seoul National University, School of MS&E, Seoul, KOREA.

The BST thin films were deposited by liquid source MOCVD with various deposition parameters. Metal organic precursors of $Ba(methd)_2$ (methd=methoxyethoxytetramethylheptanedionate), $Sr(methd)_2$, and $Ti(mpd)(thd)_2$ (mpd=methylpentanediol, thd=tetramethylheptanedionate) were dissolved in methanol. The cocktail source of BST was prepared by mixing of Ba, Sr, and Ti precursor solution with specific mole ratio. This cocktail source was vaporized and delivered into the warm wall reactor by liquid delivery system(LDS) and gaseous source was distributed by simple structure of gas injector instead of showerhead system. The oxygen gas was also supplied to the reactor directly as oxidizer through another injector. So source and O_2 gas were met in reactor. The thickness uniformity of BST on 8 inch wafers were less than 3%. The Ti composition uniformity of our films were less than the 1 at%(1σ) at stoichiometric and near stoichiometric. Because electrical properties of BST seriously depend on the Ti compositions, the control of composition uniformity of Ti is very important. Their dielectric constant was about 170 and leakage current density was lower than 10^{-7} A/cm^2 at 1V. The merit of our warm wall type reactor also will be explained in presentation. Our achievement should be applicable to the capacitor of next generation DRAM.

9:00 AM O9.3
DIELECTRIC AND FERROELECTRIC STUDIES ON $Pb_{0.9}La_{0.15}TiO_3$ THIN FILMS ON SOLUTION DERIVED RuO_2 BOTTOM ELECTRODES. S. Bhaskar, S.B. Majumder, P.S. Dobal and R.S. Katiyar, Department of Physics, University of Puerto Rico, San Juan, PR; S.B. Krupanidhi Materials Research Centre, Indian Institute of Science, Bangalore, INDIA.

Sol-Gel derived $Pb_{0.9}La_{0.15}TiO_3$ (PLT15) thin films were deposited on solution derived RuO_2/Si, RuO_2/Pt/Si and on Pt bottom electrodes. X-ray diffraction, Atomic Force Microscopy techniques were used for structural and morphological characterization of these films respectively. Dielctric, tangent loss, C-V, hysteresis, J-V J-t measurements were also carried out on these films. X-ray results established the single phase perovskite formation with no secondary phases of PLT15 thin film on these electrodes. AFM images showed surface morphology with dense uniform microstructure and low surface roughness. PLT15 thin films on RuO_2 bottom electrode showed relatively inferior ferroelectric and dielectric behavior (470, 0.040 at 100 kHz) as compared to Pt electrode. Low leakage currents (10^{-8} A/cm^2 at 10 kV/cm) and observed J-V characteristics has been attributed to poor film-electrode interface. Observed electrical and dielectric properties have been correlated with the film-electrode interface. The interface characteristics were further augumented by depth profile analysis using Auger Electron Spectroscopy. This work is supported by DAAG55-98-1-0012 and NSF-DMR 9801759 grants.

9:15 AM O9.4
EVOLUTION OF THE ELECTRO-OPTIC EFFECT WITH THE CRYSTALLINITY OF BARIUM TITANATE THIN FILMS. M. Siegert, D.J. Werder, and H.Y. Hwang, Bell Laboratories, Lucent Technologies, Murray Hill, NJ.

Ferrolectric oxide thin films are currently actively studied for a number of applications, including memory elements and electro-optic devices. A general issue is the dependence of the relevant physical properties on the length scale of crystallinity. We have studied a series of polycrystalline $BaTiO_3$ thin films grown by pulsed laser deposition, where the crystalline coherence length is systematically varied from large polycrystalline grains to amorphous by varying the substrate temperature. The structural properties have been studied by x-ray diffraction and transmission electron microscopy and compared with the evolution of various optical properties including the electro-optic effect.

9:30 AM O9.5
MICROSTRUCTURE EVOLUTION AND CRYSTALLISATION KINETICS OF SOLUTION DEPOSITED PZT THIN FILMS. Mohammed Es-Souni, André Piorra, University of Applied Sciences, Surface and Thin Films Technologies, Kiel, GERMANY.

The results of the microstructure development and crystallisation kinetics of solution deposited lead-zirkonate-titanate (PZT) and lanthanum dpoed PZT (PLZT) on different bottom electrode types including highly textured (111)-Pt, polycristalline Pt and a conductive transparent oxide are reported. It is shown that the crystallisation kenetics and the grain size depend strongly on both thin film composition and electrode type. Undoped PZT exhibits fastest kinetics on (111)-Pt. The results are analysed in terms grain boundary nucleation and growth kinetics and are interpreted in terms of interfacial reactions and interfacial stresses between the thin film and substrate.

9:45 AM O9.6
THE SIZE EFFECT OF THE POLARIZATION OF $SrBi_2Ta_{2-x}Nb_xO_9$ CAPACITOR. K. Tanaka Panasonic Semiconductor Development Company, Colorado Springs, CO; M. Azuma, Y. Shimada and T. Otsuki Semiconductor Company, Matsushita Electronics Corporation, Takatsuki, Osaka JAPAN; C.A. Paz de Araujo Symetrix Corporation, Colorado Springs, CO.

In recent years, the FeRAM integration technology is enough matures for manufacturing FeRAM commercial products using the design rule from 0.8um to 0.5um. The FeRAM technology is improved toward to realize the next generation high density FeRAM using around sub-micron design rule. However, it is known that the ferroelectric characteristic changes between the bulk crystal state and the thin film state, fabricated for the high density FeRAM. Therefore, the theoretical clarification of the high density FeRAM characteristic is become very important to realize the next generation FeRAM device on time. The size dependence of the polarization of $SrBi_2Ta_{2-x}Nb_xO_9$ (SBTN) ferroelectric capacitor was calculated in the two-dimensional capacitor system with the polarization normal to the electrodes. Two different mechanisms, the depolarization effect and the surface effect due to the change of the long-range interaction between the polarization in the vicinity of the surface and interface, were mentioned theoretically to calculate the size effect of the polarization. The free energy expression of the polarization is described as a function of position using the Landau theory with the boundary condition. The total polarization of the capacitor was described as the integration of the capacitor volume. Each expansion coefficient as a fitting parameter was calculated from the experiment data of the polarization. The simulations of the size dependence of the polarization were performed. The simulated result shows that the polarization is stable down to capacitor size 0.01um^2 and thickness 100nm. In conclusion, the ultra high density FeRAM using SBTN can be realized from the simulation of the size dependence of the polarization.

10:30 AM O9.7
HIGH RATE IN-SITU YBCO DEPOSITION: THERMODYNAMIC CONSIDERATIONS. Tsuyoshi Ohnishi, William Jo, Ann Marshall, Jeong-uk Huh, Robert H. Hammond, and M.R. Beasley, Stanford University, Laboratory for Advanced Materials, Stanford, CA; Eric Peterson, Los Alamos National Labs, Los Alamos, NM.

We are developing a high rate (up to 10 nm/s), in-situ YBCO film synthesis using an electron beam deposition method with a view

toward coated superconducting conductors for electrical power applications. Different from YBCO films grown with low rate deposition method, our films have characteristic microstructures: inclusion of large ball-shape Y_2O_3 precipitates (~100 nm), existence of surface nonstoichiometric layer, and two kinds of YBCO layers with different crystallinity underneath it, according to transmission electron microscopy, energy dispersive x-ray analysis, Br-MeOH etching, electrical transport measurements, and X-ray diffraction results. Former two features seem to indicate that the YBCO film is growing in Y deficient Ba-Cu-O liquid flux, even though we are depositing only stoichiometoric YBCO. The liquid layer is surprising considering our low oxygen pressure conditions, and we are attempting explain it based on the thermodynamics of activated oxygen in this system. By depositing a Y doped Ba-Cu-O liquid layer before the stoichiometric YBCO we are attempting to form only one kind of YBCO with high current density. Our LPE type of growth resembles Tri-phase epitaxy [1] but at order of magnitude lower pressure. The results of TPE, the liquid layer formation and decomposition of YBCO film will be discussed in the paper with the aid of reflection high energy electron diffraction. [1] M. Kawasaki, D.B. Choi, T. Ito, K.S. Yun, and H. Koinuma, *Proceedings of the third symposium on atomic scale surface and interface dynamics* **3**, (1999) 151.

10:45 AM O9.8
TAILORING MANGANESE PEROVSKITE SURFACES. C.N. Borca, Bo Xu, Takashi Komesu, Hae-kyung Jeong, M.T. Liu, S.-H. Liou, P.A. Dowben, University of Nebraska, Department of Physics and Astronomy, Lincoln, NE.

We have studied the surface composition and electronic structure of CMR perovkite thin films of $La_{0.65}Pb_{0.35}MnO_3$. Depending on the annealing treatments, the thin film surface exhibits wildly different behavior and composition. A gentle annealed surface shows 80% spin asymetry close to Fermi level, at the surface Brillouin zone center, and a Curie temperature of 335 K, while a heavy annealed surface has a reduced polarization (45%) and a nonmetal-metal transition temperature of 245 K. The composition of the two types of surfaces was analyzed using angle dependent X-ray photoemission, and the unoccupied bands were assigned by comparing the X-ray absorbtion with inverse photoemission spectra. As expected, the high polarization near the Fermi level is a consequence of the Mn atoms which contributed to the majority of the magnetic moment. Tailoring surfaces of complex CMR compounds may lead to improvements in device performances. The current results shed considerable light on the device performance of the CMR perovskites in tunnel magneto-resistive junctions and spin valves in the thin film limit.

11:00 AM O9.9
EVOLUTION OF THE MICROSTRUCTURE, GROWTH STRESS AND STIFFNESS OF ALUMINA THIN FILMS DURING VAPOR DEPOSITION. Joris Proost and Frans Spaepen Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA.

The stress in alumina thin films, e-beam deposited on a silicon or sapphire substrate, was monitored in situ with measurements of the substrate curvature. At 400C, the growth stress is tensile, with a magnitude of 230 MPa for thicknesses up to 700 nm; at higher thicknesses, the magnitude decreases. Interruption of the deposition causes no change in the curvature. Thermal cycling up to 450C results in reversible curvature changes, due to thermal stresses. From these, the biaxial modulus and coefficient of thermal expansion of the films could be determined. The biaxial modulus decreases continuously with thickness, from a value of 310 GPa at 100 nm to 65 GPa at 2000 nm. This decrease correlates with a decrease in density, on the order of 15%. The increased porosity is accompanied by increased surface roughness, observed directly by AFM and SEM, as well as by interferometry on the reflections of the curvature measurement. A quantitative model for the relation between thickness, density, stiffness and growth stress is being developed.

11:15 AM O9.10
PHASE FIELD MODELING OF ELECTRODEPOSITION
J.E. Guyer, W.J. Boettinger, and J.A. Warren Metallurgy Division, National Institute of Standards and Technology, Gaithersburg, MD.

We will present a novel computational model of electroplating, using the phase field method. This method abandons the mathematical artifice of a sharp (two dimensional) transition between liquid and solid. This sharp transition requires tracking of the position and shape of the liquid-solid interface and the application of boundary conditions at a surface whose shape is part of the solution, a difficult task for all but the simplest geometries. Phase field calculations, on the other hand, define a variable and a corresponding governing equation to describe whether a material is solid or liquid as a function of both position and time. With the addition of conventional solute diffusion equations, the evolution of complex growth patterns and the equations for the dynamics of the process can be solved without tracking the liquid-solid interface. The numerical method is a finite difference technique on a uniform mesh, making implementation straightforward for the novice programmer. This method allows us to treat the complex geometry, including void formation, that occurs during plating in vias and trenches for on-chip metallization. It also provides for a proper treatment of curvature effects on the overpotential. The phase field technique has been successfully applied to such complex morphologies as the cellular breakdown of high-velocity directional solidification and dendrite formation under convective flow, but this is the first time that phase field modeling has been applied to electrochemical problems. This work was motivated by the mathematical analogy between the governing equations of solidification dynamics and electroplating dynamics but it is not surprising that we find significant differences between the two systems. Indeed, the inherent non-linear kinetics in electrodeposition is far different from solidification, where problems are generally well-modeled with linear kinetics. We will present different techniques for deriving these non-linear phase field equations and the consequences of each.

11:30 AM O9.11
GROWTH AND CRYSTALLOGRAPHIC ORIENTATION OF ELECTROMIGRATION-INDUCED HILLOCKS IN ALUMINUM INTERCONNECTS. J.A. Nucci, C.A. Volkert, A. Straub and E. Arzt, Max Plank Institut für Metallforschung, Stuttgart, GERMANY.

Hillocks form in metal films due to compressive stress generated either by thermal cycling or electromigration. Understanding how they grow may help to elucidate possible mechanisms for atomic motion and stress relief in thin films. In this study we have carefully investigated the morphology and crystallography of electromigration-induced hillocks, from which their growth mechanism can be determined. Structures consisting of unpassivated, Al segments of various lengths and connected by a continuous underlying TiN layer were electromigration tested at 250°C and 1 MA/cm^2. After two hour intervals, the test was interrupted and hillock orientations were investigated using electron backscattering diffraction. Finally, the microstructure of the hillocks was extensively characterized using atomic force microscopy, field emission SEM, TEM, and focussed ion beam (FIB) microscopy. FIB cross sections revealed that hillock growth occurred by epitaxial addition of Al atoms at the Al/TiN interface. As the hillocks grew, their normal directions rotated away from $< 111 >$ texture accompanied by rigid body rotation of the entire grain about the same axis, as determined from the surface morphology. Such growth is consistent with atomic diffusion along grain boundaries and down into the bottom interface, which pushes up and rotates the hillock as it grows.

11:45 AM O9.12
Transferred to O2.2/R2.2

SESSION O10: SILICIDES AND ORGANIC THIN FILMS: PULSED LASER DEPOSITION

Chairs: Jacques G. Amar and John E. Sanchez
Friday Afternoon, April 20, 2001
Salon 7 (Marriott)

1:30 PM O10.1
SELF-ASSEMBLED SILICIDE NANOWIRES GROWN ON SILICON (001). Yong Chen, Douglas A.A. Ohlberg, R. Stanley Williams, Hewlett-Packard Laboratories, Palo Alto, CA.

Many silicides have an asymmetric lattice-mismatch to Si(001) host substrate, which can break the growth symmetry and lead to the self-assembled epitaxial growth of silicide nanowires. Four silicides, ScSi2, ErSi2, DySi2, and GdSi2 with different lattice-mismatches have been chosen to grow on Si(001). The widths and the lengths of the nanowires were in the range of ~3-15 nm and ~100-1000 nm, respectively, for different lattice-mismatches and growth conditions. The larger lattice-mismatches along the width direction led to the narrower wires, and the smaller lattice-mismatches along the length direction led to the longer lengths. This method provides an effective way to fabricate one-dimensional quantum system with desired sizes for novel physical properties.

1:45 PM O10.2
LOW TEMPERATURE HETEROEPITAXIAL TITANIUM SILICIDE PHASES IN 3 nm ISLANDS SEEDED ON (7x7)Si(111) TEMPLATES AT T * 500°C. N. Herbots, J.M. Shaw, M. Liger, M.P. Grams, D.J. Smith, Dept of Physics and Astronomy, Arizona State University, Tempe, AZ.

3-nm wide titanium silicide islands are formed on (7x7)Si(111)

templates below 500 degree Celsius by Combined Ion and Molecular Beam Deposition (MBE) in order to investigate the possibility of obtaining a periodic array of titanium silicide quantum dots seeded by the 2. 8 nm (7x7) unit cells. These temperatures are compatible with quantum dot processing, by minimizing surface diffusion. After growth room temperature deposition of Si, followed by low temperature oxidation and rapid thermal oxidation is used to further isolate and encapsulate the dots to protect them from oxidation in air for electrical measurements while working on the NSF seed. Indeed, if exposed to air without encapsulation, the dots tend to vanish. Two distinct titanium silicide phases are nucleated below 800 K. The first silicide phase formed is found to be close but not lattice matched to Si(111) by RHEED diffraction. Plan-view HRTEM shows that this initial phase facets in the characteristic triangular shape of a periodic island nucleated on the (7x7)Si(111) unit cell. The second silicide phase has about twice the lattice constant of Si(111) and facets in a more complex polygonal shape. Interference fringes in HRTEM imaging is observed within the two kinds of islands confirms the RHEED findings on lattice constants. Unit cell szie in the second phase appears to be close the C54 titanium disilicide phase along the c-axis. Results from Electrical measurements, high resolution Medium Energy Ion Scattering (MEIS) combined with Channeling and Blocking and Atomic Force Microscopy results will also be discussed. Support by the National Science Foundation under grant DMR-9632635 is here acknowledged.

2:00 PM O10.3
DYNAMICS OF SHAPE TRANSITION OF EPITAXIAL $TiSi_2$ ISLANDS ON Si(111) SURFACES. Woochul Yang, R.J. Nemanich, North Carolina State Univ, Dept of Physics, Raleigh, NC.

The evolution dynamics of the shape and size of nanoscale $TiSi_2$ islands on Si(111) surfaces is explored using ultra-violet photoelectron emission microscopy(UV-PEEM). *in situ* continuous deposition at elevated temperatures and real-time monitoring of the growth of the islands can allow us to study the consecutive shape evolution of the individual islands. The islands were prepared by *in situ* Ti deposition of ~1ML at room temperature followed by annealing to 1150°C. During annealing, we observed island coarsening (both ripening and coalescence) where smaller islands evolved into larger islands and the surface morphology displayed a dilute island distribution. In addition, high temperature deposition of Ti for further grwoth of the islands led to increased size of the individual islands without new island nucleation or island disappearance. In particular, a spontaneous shape transition of the islands was observed in which the islands are initially symmetric and then develop into elongated structures with high aspect ratios greater than 85:1 (length:width). However, the width and height, determined at the initial transition stage, remain constant with increasing length. Also, 3d-AFM images of the elongated islands revealed two different type shapes: Wider islands with a flat top and trapezoidal cross-section, and narrow islands with a sharp top and triangular cross-section. We propose that the different shapes are related to strain relaxation in the individual islands.

2:15 PM O10.4
INFLUENCE OF DENDRIMER INTERLAYER ON METAL ADSORPTION. A. Rar, G. Wei, F.T. Xu, J.A. Barnard, The Center for Materials for Information Technology, M. Curry, S.C. Street, Department of Chemistry, The University of Alabama, Tuscaloosa, AL.

Si wafers covered with a native oxide were used as substrates for the growth of thin metal layers, mediated by a self-assembled monolayer of amine-terminated poly(amidoamine) (PAMAM) dendrimers (generation (G) 4, 8 and 10). The films were studied using a combination of XPS, XRR (x-ray reflectivity), AFM, and nanoindentation. It was shown recently [1], that for an inert metal, such as Au, metal atoms penetrate into G8 dendrimer, leading to improvements in film quality. When dendrimers are used as an interlayer the hardness Au increased two-fold. The surface roughness decreased by three-fold, and better adhesion was noted. Penetration should be less pronounced for active metals such as Al, Co, Cr and Cu, because of increased chemical activity with the outermost amine terminal groups. The outer shell of the dendrimers become more dense with increasing generation number, thus penetration of the deposited metals should follow the trend G4>G8>G10. This is confirmed by XPS, and related to observed mechanical properties and morphology of the deposited films. Apparently, for the more active metals forming a bilayer system gives a mechanically softer film as a result of yielding of the dendrimer interlayer during nanoindentation. 1. A. Rar, J.N. Zhou, A. Bennett, W.J. Liu, J. Barnard, and S.C. Street, Dendrimer - Mediated Growth of Very Flat Ultrathin Au Films, Appl. Surf. Sci., in press.

2:30 PM O10.5
INVESTIGATION OF MATERIAL FLOW ON INSCRIBING A POLYMER SURFACE GRATING PROBING X-RAY AND VIS LIGHT SCATTERING. Thomas M. Geue, Oliver Henneberg, Marina Saphiannikova, Ullrich Pietsch, University of Potsdam, Institute of Physics, Potsdam, GERMANY; Almeria Natansohn, Queen's University, Department of Chemistry, Kingston, ON, CANADA; Paul Rochon, Royal Military College, Department of Physics, Kingston, ON, CANADA; Ken Finkelstein, Cornell University, CHESS, Ithaca, NY.

Surface relief patterning on amorphous polymer films containing azobenzene-side chains can be performed by holographic exposure with visible light of about 488 nm at room temperature. In order to understand the dynamics of the induced material flow we performed in-situ time-resolved coherent x-ray and VIS light scattering measurements at exposure with a holographic pattern obtained using circularly polarized light of 40 mW/cm^2. The films under investigation were made from a series of polar azobenzene side-chain homopolymers. The efficiency of grating formation is probed by the time development of the diffracted first-order grating peak intensities. While the VIS signal increases continuously during continuous holographic exposure, the x-ray grating peak intensity reaches a maximum after about 60 s and decreases thereafter. Similar measurements during short time exposure show that the maximum of the x-ray signal depends of the pulse length of the inscribing light. An analysis of the time evolution of the VIS scattering reveals the existence of sequential elastic and plastic processes during exposure. Both experiments can be explained qualitatively by assuming the formation of a density grating in addition to the surface relief patterning. Our assumption are validated by model calculations using a finite element (FE) approach including a sinusoidal force distribution accompanied by visco-elastic flow.

2:45 PM O10.6
VERTICAL LAMELLAE IN THIN FILMS OF DIBLOCK COPOLYMERS. Detlef-M. Smilgies, Cornell Univ, CHESS, Ithaca, NY; Christine Papadakis, Peter Busch, Univ of Leipzig, Dept of Physics and Geosciences, Leipzig, GERMANY; Dorthe Posselt, Roskilde Univ., Dept. of Mathematics and Physics, Roskilde, DENMARK.

Polymer coatings have great technological importance for e.g. processing of integrated circuits and optical coatings. Hence investigations of the microstructure of polymer blends and block copolymers has become an active field of research in recent years. Recently we have found that symmetric di-block co-polymer films of polystryrene-polybutadien prepared by spin-coating onto Si-wafers can form lamellae oriented perpendicular to the substrate surface, provided the molecular weight of the polymer is above 92 kg/mol. Polymers having molar masses below 22 kg/mol form the well-known horizontal lamellae parallel to the surface. We have studied such films using a combination of atomic force microscopy (AFM) as well as synchrotron-based x-ray reflectivity (XR) and grazing-incidence small angle scattering (GISAXS. Our AFM studies were invaluable for the optimization of sample preparation procedures. However, the internal structure of the films is not accessible to this probe. Hence we complemented our studies with x-ray scattering techniques, XR to probe the normal density correlations in the film, and GISAXS to probe the lateral structure of the films. In order to enhance the scattering contrast, the butadien blocks were stained with osmium tetroxide. We studied such films at various thicknesses and molar weights. Films with molar masses between 92 to 183 kg/mol show XR and GISAXS scattering indicative of the lamellae continuing all the way from the surface to the substrate. Most interesting signatures had films of intermediate molar weights in the range of 55 to 70 kg/mol: The AFM pictures show an inhomogeneous surface with some onion-like regions of vertical lamellae inbetween unstructured areas. Consistent with this finding, XR and GISAXS indicate some fraction of parallel lamellae and a curving of the vertical lamellae, respectively. Hence, using a combination of AFM, XR, and GISAXS a full characterization of the microstructure of polymer thin films can be achieved.

3:30 PM O10.7
THE INITIAL GROWTH AND THE CHARACTERIZATION OF SEMICONTINUOUS METAL FILMS BY PULSED LASER DEPOSITION. S.K. So and N.H. Cheung, Department of Physics, Hong Kong Baptist University, Kowloon Tong, Hong Kong, CHINA.

Extremely thin (1-5 nm) copper and gold films were prepared by pulsed laser deposition (PLD) on glass, MgO and sapphire substrates. [1] The resistivity and transmittance of these metal films during growth were measured as a function of film thickness. In contrast to vacuum evaporated thin films, a sharp insulator-to-metal percolation region can be identified for nearly all metal films prepared by PLD. Concomitant with this transition, the transmittance exhibits a dip. As a result, the dynamics of percolation of very thin metal films can be independently monitored by means of in situ resistivity and transmittance measurements. The occurrence of percolation threshold

is found to be independent of the incoming flux of the metal atoms ejected from the PLD target. Slowing the moving metal atoms by helium tends to delay the onset of percolation. In contrast, growing the metal films on atomically flat surface such as sapphire or MgO favors the early onset of the percolation. Under favorable conditions, PLD Cu or Au films as thin as 1.5 nm would percolate, and the threshold is at least a factor of 3 better than evaporated thin films. At about 5 nm, the conductivity would reach 30% of the bulk value. It is expected that by controlling various PLD parameters, the optical and electrical properties of semicontinuous metal films can be engineered. The physics of these metal films is also under investigation. [1] S.K. So, H.H. Fong, C.F. Yeung, and N.H. Cheung, Appl. Phys. Lett. 77, 1099 (2000).

3:45 PM O10.8
PULSED LASER DEPOSITION OF DENSE PEROVSKITE FILMS ON MACROPOROUS SUBSTRATES FOR GAS SEPARATION APPLICATIONS. Edward A.F. Span, Dave H.A. Blank, H. Rogalla, University of Twente, Dept. of Applied Physics, Enschede, THE NETHERLANDS; Marco v.d. Haar, Henny J.M. Bouwmeester, Henk Verweij, University of Twente, Dept. of Chemical Engineering, Enschede, THE NETHERLANDS.

Pulsed-laser deposition (PLD) was investigated for depositing thin films of the mixed ionic-electronic conducting perovskite $La_{1-x}Sr_xCoO_3$ (LSCO) on macroporous a-Al_2O_3 substrates (pore size ~100 nm) for use as oxygen separation membranes. It is demonstrated that reduced oxygen-pressure deposition at room temperature leads to smooth, uniform and dense films that are completely gas-tight to nitrogen gas whereas films deposited at high oxygen pressures are rough, granular and porous. Moreover, we report on the deposition of LSCO films on coarse-porous LSCO substrates (pore size >1 um) in an attempt to develop all-perovskite oxygen separation membranes. Prior to the deposition, the substrate surfaces were chemically etched or modified with a dip-coating. It is found that, under the right deposition conditions, continuous and non-porous films with excellent textures can be grown on these types of substrates. First oxygen permeation measurements reveal that the films show very high oxygen fluxes at temperatures between 700 and 1000 degree Celcius.

4:00 PM O10.9
HETEROEPITAXIAL GROWTH OF TAN ON MgO(001) AND TiN(001)/Si(001) BY PULSED LASER DEPOSITION. H.Y. Cheung and K.H. Wong, Department of Applied Physics and Materials Research Centre, Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, PR CHINA.

Epitaxial TaN(001) films have been successfully grown on MgO(001) single crystal and TiN(001) buffered Si(001) substrates by pulsed laser deposition method. Crystalline TaN layers of about 100 nm thick were deposited under a base pressure of 5×10^{-6} Torr and at substrate temperatures ranging from 500°C to 700°C. X-ray diffraction results suggested that stoichiometric TaN films with cube-on-cube $(001)_{TaN} \| (001)_{MgO}$ heteroepitaxy are obtained in this temperature range. Plan-view and cross-sectional electron microscopy analysis revealed excellent structural quality and sharp interface boundary. TaN films grown on TiN(001) buffered Si(001), however, showed a mixture of TaN_x (with $x \geq 1$) components. Although the (001)-orientated TaN is always present prominently, the nitrogen deficient TaN_x components are often co-exist in the films and show up as a very broad peak in the X-ray diffraction profile. Their magnitude and position change with the deposition temperature and show a strong dependence on the growth condition of the TiN buffer layers. Stoichiometric and single phase TaN(001) films can only be obtained in a narrow temperature window at around 550°C and heteroepitaxial relation $(001)_{TaN} \| (001)_{TiN} \| (001)_{Si}$ has been demonstrated.

4:15 PM O10.10
SYNTHESIS OF TIN OXIDE THIN FILMS BY PULSED LASER DEPOSITION USING SnO_2 TARGETS. Yoshiaki Suda, Hiroharu Kawasaki, Kazuya Doi, Jun Namba, Sasebo National College of Technology, Department of Electrical Engineering, Sasebo, Nagasaki, JAPAN; Kenji Wada, Department of Chemistry and Biotechnology, Sasebo, Nagasaki, JAPAN; Kenji Ebihara, Tamiko Ohshima, Kumamoto University, Department of Electrical and Computer Engineering, Kumamoto, JAPAN.

Tin Oxide (SnO_2) has been utilized as a gas sensing material, because it shows an electric conductivity change in contact with flammable gases. SnO_2 thin films have been grown on Si(100) and Al_2O_3 substrates by pulsed Nd:YAG (532nm) and KrF excimer (248 nm) laser deposition method using SnO_2 targets. The effects of substrate temperature and oxygen gas pressure on the properties of the SnO_2 thin films are discussed. Surface morphology and structure of the films have been obtained by field emission scanning electron microscopy (FE-SEM), atomic force microscopy (AFM) and glancing-angle X-ray diffraction (GXRD) measurement. GXRD showed that, with increasing oxygen gas pressure, the almost amorphous microstructure transformed into a crystalline SnO_2 phase and preferred orientations varied from (101) to (110) on Si(100). This result suggests that oxygen gas pressure affects the phase formation, crystalline structure and preferred orientation of the films. Gas sensing properties of SnO_2 thin films by PLD method are also investigated over the temperature range 473K -873K, using H_2 or CH_2 as test gases.

4:30 PM O10.11
$Pb(Mg_{1/3}Nb_{2/3})O_3$ - $PbTiO_3$ RELAXOR THIN FILMS BY PULSED LASER DEPOSITION. Rasmi R. Das, W. Pérez, Ram S. Katiyar and S.B. Krupanidhi[a]; Physics Department, University of Puerto Rico, San Juan PR; [a]Materials Research Center, Indian Institute of Science Bangalore, INDIA.

The relaxor composition $(PbMg_{1/3}Nb_{2/3}O_3)_{0.9}$ -$(PbTiO_3)_{0.1}$ thin films were deposited by PLD on $Pt/TiO_2/SiO_2/Si$ substrates. Several growth parameters were varied to optimize the film properties, which include; substrate temperature, ablation pressure, laser fluence and the annealing temperature. Pure perovskite phase in polycrystalline thin films grown at different substrate temperatures (300 - 650°C) was obtained after the films were subjected to an annealing at 850°C. Films were characterized in terms of structure (XRD), phase identification (micro-Raman), morphology (AFM) and electrical behavior. Films with near complete perovskite phase exhibited a dielectric constant of about 2000 and a dissipation factor of about 0.02. Detailed results on structural and electrical studies will be discussed in close correlation with the processing conditions.

4:45 PM O10.12
PULSED-LASER DEPOSITION OF TiNi SHAPE MEMORY ALLOY THIN FILMS AT DIFFERENT TEMPERATURES. X.Y. Chen, Y.F. Lu, Z.M. Ren, S. Zhu, J.P. Wang, T.Y.F. Liew, NUS, Department of Electrical and Computer Engineering, Singapore, SINGAPORE.

Thin films of TiNi shape memory alloy (SMA) have been prepared by pulsed-laser deposition (PLD) at different substrate temperatures. The stoichiometry, deposition rate, and crystallinity of the deposited films were characterized by X-ray photoelectron spectroscopy (XPS), surface profile measurements, and X-ray diffraction (XRD). The transformation behavior and crystallization temperatures were investigated by differential scanning calorimetry (DSC). It is found that the deposition rates are of the order of 10-2 nm per pulse. The Ni content ranges from 46.7 to 52.0 at%. The film deposited at a substrate temperature of 600°C has a poly-crystalline structure and austenite is the major phase. The martensitic transformation temperature of the annealed Ti-51.5 at% Ni thin film is determined to be ~20.8°C. The crystallization temperatures of the amorphous films are around 430°C. It can be concluded that the substrate temperature plays an important role in the composition control and the crystallization of the films.