SYMPOSIUM N

Current Issues in Heteroepitaxial Growth–Stress Relaxation and Self Assembly

November 26 – 29, 2001

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* Invited paper

SESSION N1: EARLY STAGES AND FUNDAMENTAL PROCESSES OF HETEROEPITAXY
Chairs: Anthony G. Cullis and Vivek B. Shenoy
Monday Morning, November 26, 2001
Room 306 (Hynes)

8:30 AM *N1.1
ISLAND GROWTH AND THE STRANSKI-KRASTANOW TRANSITION. Anthony Cullis, Dept of Electronic and Electrical Engineering, University of Sheffield, Sheffield, UNITED KINGDOM; Thomas Walther, Institut fuer Anorganische Chemie, Universitaet Bonn, Bonn, GERMANY.

Epitaxial semiconductor layer growth is a vital component of electronic device technology and, in particular, heteroepitaxy is increasingly employed to provide the benefits of varying band structure within individual devices. However, the lattice mismatch between the different layer components can determine the way in which layer epitaxy proceeds and, in the large mismatch regime, the Stranski-Krastanow 2D to 3D transition generally takes place early in the layer growth process leading to the formation of arrays of growth islands. Indeed, the manner in which this transition occurs is of considerable importance since the nature of the islands formed controls their exploitation as, for example, quantum dots in electronic device structures. This presentation will consider the evidence available in a number of semiconductor epitaxial systems and will link the occurrence of the transition to fundamental growth processes during the early layer growth phase. Furthermore, while islands are forming, the way in which their internal composition evolves is also of special importance because this determines their electronic properties, again of direct relevance to electronic device applications. Recently, measurements have been made upon individual growth islands and these provide direct evidence regarding internal composition variations. The various available results will be reviewed.

9:00 AM N1.2
ROLE OF PRECURSOR FORMATION IN THE GROWTH OF InAs/GaAs(001) QUANTUM DOTS. Tim Jones, T.J. Krzyzewski, G.R. Bell, P.B. Joyce, Centre for Electronic Materials and Devices and Dept of Chemistry, Imperial College, London, UNITED KINGDOM.

The formation of InAs quantum dots (QDs) on GaAs(001) surfaces is of great current interest due primarily to the opportunity of producing novel optoelectronic devices but also because of the more general question of 'self-organisation' in epitaxial growth. The transition from a 2D layer-by-layer growth mode to 3D island growth occurs very rapidly in this system. It also appears that the number density of QDs is essentially determined at this stage in the growth, and is reduced by lowering the InAs deposition rate or raising the growth temperature. We have used scanning tunnelling microscopy (STM) to monitor the growth of InAs on GaAs(001) at coverages close to the critical coverage (θ_{crit}). Direct STM evidence, at much better resolution than previously reported, is provided for the existence of 3D precursors. They have an ill-defined shape and height 6-12 $\AA$ (2-4 ML) and an average volume of $\sim$400 atoms, and develop extremely rapidly (within 0.05 ML of θ_{crit}) into large, mature QDs with an average volume of 10000-150000 atoms. The active role of 2D, 1 ML-high platelets, which have been suggested to act as precursors in QD formation, is limited to that of a step edge. Further more we find no evidence for a re-entrant 2D-3D morphology transition at coverages below θ_{crit}. The nature of the transition to 3D growth is discussed in terms of surface reconstruction changes, In adatom densities and strain energy.

9:15 AM N1.3
SIMULATION OF MECHANISMS IN STRAINED SILICON GERMANIUM EPITAXY. Richard J Wagner, Erdogan Gulari, Dept of Chemical Engineering, University of Michigan, Ann Arbor, MI.

Heteroepitaxy of silicon germanium produces a strained crystal that can self-assemble into electronically interesting structures such as quantum dots. We have developed simulations to study the mechanisms of this complex process. Equilibrium and kinetic Monte Carlo simulations are used to examine the energetics and time evolution of the growth process. Molecular dynamics simulations were performed to uncover reaction pathways important to growth. The model is based on an interatomic potential that mimics the directionality of bonding and size mismatch in the diamond lattice of SiGe. Strain in the growing crystal is derived from the potential and affects diffusion of atoms on the surface. The distribution of this strain and its impact on bond energies are found. The relation of self-assembly to material composition is also examined. Our goal is to eventually permit engineering of desired microelectronic structures through control of material composition and growth conditions.

9:30 AM N1.4
ADATOM-DENSITY KINETIC MONTE CARLO(AD-KMC):A NEW METHOD FOR FAST GROWTH SIMULATION. Lorenzo Mandreoli, Joerg Neugebauer, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, GERMANY.

We have developed a new method (AD-KMC) to perform growth simulations which combines the advantages of kinetic Monte Carlo (direct use of microscopic parameters/processes) with continuum equations (which are very fast). The main idea is to directly calculate the time evolution of the adatom density, rather than following the trajectory of each individual adatom as done in KMC. The adatom density is obtained by solving directly the master equation and taking all microscopic processes into account. In this way the simulation time step is no longer limited by the jump rate of the adatoms but by the time scale of the events modifying the surface (island nucleation, attachment at steps) making this method fast even at high temperature. To test the method, we have compared nucleation density, island size distribution, island shapes for various systems with conventional KMC-techniques. Finally, we show how this method can be applied to describe complex systems such as self-organization in V-grooves or lateral overgrowth.

9:45 AM N1.5
A SIMPLE GENERIC METHOD FOR PREDICTING THE EFFECT OF STRAIN ON SURFACE DIFFUSION. Feng Liu, Univ of Utah, Dept of Materials Science and Engineering, Salt Lake City, UT; D.J. Su, X.G. Gong, Chinese Academy of Science, Institute of Solid State Physics, Hefei, CHINA.

We show, by first-principles calculations, that the effect of external strain on surface diffusion is *inherently* correlated with the intrinsic surface stress induced by the adatom along its diffusion pathways. We demonstrate a simple generic method for *a priori* predicting quantitatively how an external strain will change surface diffusion on any given surface, based on calculations of surface stress tensors of the unstrained surface.

10:30 AM *N1.6
ATOMIC MECHANISMS AND CONTINUUM MODELING OF HETEROEPITAXY. J. Tersoff, IBM T.J. Watson Research Center, Yorktown Heights, NY.

Our understanding of heteroepitaxial growth and stress relaxation is largely based on continuum models. Atomistic models are potentially more realistic; but in practise it is not feasible to use these to address the growth regimes relevant for technological materials. Yet standard continuum models neglect many important effects of atomic structure; and these effects are increasingly important with the trend toward growth at lower temperatures. A generalized continuum treatment can incorporate some of the effects that are usually omitted. Results of such a treatment include running-wave instabilities on vicinal strained layers, and suppression of stress-induced instabilities by the strain-dependence of kinetic "rate constants".

11:00 AM N1.7
KINETIC VERSUS STRAIN-INDUCED GROWTH INSTABILITIES ON VICINAL Si(001). J. Myslivecek, C. Schelling, G. Springholz, F. Schäffler, University Linz, AUSTRIA; B. Voigtländer, Forschungszentrum Jülich, GERMANY; P. Smilauer, Czech Academy Sci., Prague, CZECH REPUBLIC.

The step-bunching growth instability on the surface of SiGe/Si(001) heterostructures and superlattices has long been attributed to a strain-driven equilibrium effect. Recently, we could show [PRL 83, 995 (1999)] that the same ripple morphology develops under kinetic growth conditions during Si homoepitaxy on slightly vicinal (001) surfaces. Meanwhile, we mapped out a large range of the multi-dimensional growth parameter range and found no indications for strain-driven step bunching in the Si/SiGe heterosystem. To identify the microscopic origin of this evidently kinetic effect, we performed large-area AFM experiments, atomically resolved in-situ STM measurements and kinetic Monte Carlo simulations. In the step-bunching regime we find strong evidence for the presence of an asymmetric step edge barrier that prevents adatom attachment from the lower terrace. This barrier behaves in every respect inverse to the usual Ehrlich-Schwoebel (ES) barrier and causes step bunching in the step-flow regime. At lower temperatures the simulations show that 2D island nucleation suppresses step bunching, in agreement with the experiments. At high temperatures the surface approaches the well-known, flat equilibrium morphology, which consists of evenly spaced monoatomic height steps. Both experiments and simulations show that the surprisingly abrupt transition from the step-bunching regime to the equilibrium morphology within a few ten K is correlated with the rather narrow temperature range where double atomic height DB steps are kinetically formed. This suggests that an inverse ES barrier on Si(001) is associated with DB steps only.

11:15 AM N1.8
ORIGIN OF THE GROWTH INSTABILITIES: COMPARISON BETWEEN Si/Si AND SiGe/Si. Isabelle Berbezier, Antoine Ronda, Alina Pascale, Alain Portavoce, Fabien Volpi, Campus de Luminy, Marseille, FRANCE.

The evolution of growth instabilities during epitaxial growth on Si surfaces has been of increasing interest over the past years for fundamental and application reasons. Indeed, as a function of temperature, surface orientation or impurity concentration, Si and SiGe layers can present highly corrugated surfaces with sinusoidal-like shape induced by step bunching or step meandering processes. Such morphologies can be used as template layers for self-assembling of Ge quantum dots. The scaling law describing the evolution of the instability amplitude and wave-length with various parameters is discussed. We show that both the onset of the instability and its development are highly dependent on the substrate orientation, the step density, the level of stress and the temperature.

11:30 AM N1.9
NUCLEATIONLESS GROWTH OF STEPPED-ISLANDS IN STRAINED HETEROEPITAXY. V.B. Shenoy, L.B. Freund, Division of Engineering, Brown University, Providence, RI.

It is generally believed islanding in strained heteroepitaxy of alloy films proceeds via nucleation and growth. Recent experiments have revealed that islanding in alloy films takes place through a stress driven instability mechanism that does not involve nucleation. We investigate the energetics of these islands by viewing them as "stepped mounds". We find that the stress induced interactions between the steps that constitute the mounds can result in a growth mode without nucleation above a certain critical value of epitaxial stress. Furthermore, the existence of this nucleationless instability depends on the sign of the epitaxial stress i.e, if it is tensile or compressive. Comparison of our model with experimental observations are reported.

11:45 AM N1.10
DISCRETIZED CONTINUUM MODEL OF STRAINED HETEROEPITAXY. Geoffrey D. Simms, Mark F. Gyure, HRL Laboratories, Malibu, CA; Alexander C. Schindler, Dimitri D. Vvedensky, Blackett Laboratory, Imperial College, London, UNITED KINGDOM; Russel E. Caflisch, Cameron Connell, UCLA, Dept of Applied Mathematics, Los Angeles, CA.

A discrete lattice model based on the full equations of linear continuum elasticity is used to examine effects of inhomogeneous strain in thin heteroepitaxial layers. The elastic coupling of surface features such as islands, or steps on a vicinal surface, to substrate features is found to be substantial. Using model parameters consistent with Si-Ge heterostructures, for films up to a few monolayers thick, the coupling is strong enough to pin surface steps to substrate steps. Such pinned steps remain fixed when annealing in zero adatom flux. For thicker films, the interaction is still sufficient to strongly impede strain-induced step bunching. The pinning energy and time scaling of step-bunching as a function of film thickness and substrate misfit is addressed.

SESSION N2/AA3: JOINT SESSION
HETEROEPITAXY AND SELF ASSEMBLY
Chairs: Frances M. Ross and Michael J. Aziz
Monday Afternoon, November 26, 2001
Room 306 (Hynes)

1:30 PM *N2.1/AA3.1
CONTROLLING THE GROWTH OF SELF-ASSEMBLED NANOSTRUCTURES DURING HETEROEPITAXY. F.M. Ross, IBM T.J. Watson Research Center, Yorktown Heights, NY.

Control of the shape, size and especially the placement of self-assembled nanostructures during heteroepitaxial growth remains a significant challenge to using these structures in novel devices. Precise control of island size and shape is required for good electronic properties, and islands must be accurately positioned in devices such as cellular automata and single electron transistors. In this presentation we will describe approaches to the control of nanoscale structures, in particular self-assembled islands, based on an understanding of the heteroepitaxial growth process obtained from real-time observations made during growth. Video-rate observations made during deposition of Ge and SiGe on Si(001), a model system which has features in common with other strained layer semiconductor systems, allow us to model island growth as a modified coarsening process and therefore to suggest conditions which optimize the size distribution. Furthermore, by observing island shape changes in real time during growth we can understand the sequence of shapes which form and relate this to the size distribution. Island placement remains the most intriguing factor to control because of the apparently random nucleation, although pre-nucleation fluctuations visible during growth experiments may provide a clue to the important processes. Since island development is dominated by competition between strain and surface energy, modulating the surface strain has a dramatic influence on nucleation: it is well known, for example, that nucleation is enhanced at the relaxed tops of mesa structures. Here we will describe nucleation in the strain field of buried dislocations which provides an opportunity for quantitatively determining the effect of stress without any associated surface topography. Methods for patterning the dislocations will be considered. We will also describe in situ modification of the substrate surface using a focused Ga ion beam, and describe the effect of such modification on the nucleation of nanostructures.

2:00 PM N2.2/AA3.2
SELF ASSEMBLING AND ORDERING OF Ge/Si QUANTUM DOTS ON FLAT AND NANOSTRUCTURED SURFACES. Nunzio Motta, Anna Sgarlata, Adalberto Balzarotti, University of Rome "Tor Vergata", Dept of Physics and INFM, Rome, ITALY; Federico Rosei, Univ Aarhus, Inst. of Physics and Astronomy and CAMP, Aarhus, DENMARK.

We have followed the self assembling in real time of Ge islands on flat and nanostructured Si surfaces. By the use of a variable temperature STM several movies of the wetting layer formation up to the nucleation of 3D islands have been recorded. The shape of the islands is driven by the substrate symmetry, resulting in square based pyramids for Si(100), and truncated tetrahedra for Si(111). These islands evolve into multifaceted nanocrystals, which are stable on Si(100), and transform into atoll-like structures on Si(111). Consistent erosion is found in the substrate surrounding the islands, indicating the presence of a high strain field which act as a driving force for removing the atoms from the wetting layer. The way in which the substrate is eroded can be explained by the phenomenon of the surface melting due to the high pressures determined by the heteroepitaxy, as recently calculated. However, in order to explain the atoll formation, a substantial intermixing reaching the core of the island should be assumed. This intermixing has been measured by our group by the XAFS technique, and the results are in good agreement with the first principles calculation performed by the group of Kelires. The actual shape of the Si(111) surface (step bunching) influences greatly the location of the growing structures, which nucleate firstly on the steps and after on the terraces, forming ordered arrays of islands, whose spacing and dimensions are controlled by the diffusion coefficient as a function of the terrace size. Alternatively, it is possible to nucleate array of ordered dots, controlling also their dimensions, by creating artificial defects on the surface. This way is actually one of the most promising for the future applications.

2:15 PM N2.3/AA3.3
SELF ORGANIZED ARRAY OF QUANTUM NANOSTRUCTURES VIA A STRAIN INDUCED MORPHOLOGICAL INSTABILITY. David Montiel[a], Judith Müller[b], Eugenia Corvera Poiré[a].
[a] Departamento de Física y Química Teórica, Facultad de Química, UNAM. Ciudad Universitaria, México, DF, MEXICO; [b] Institut-Lorentz, Universiteit Leiden, Leiden, THE NETHERLANDS.

We study the strain induced morphological instability at the early stages of heteroepitaxial growth on a vicinal substrate with regularly spaced steps. We perform a linear stability analysis and determine for which conditions of coverage a flat front is unstable and for which conditions it is stable. We discuss the effect of step energy and the effect of external flux. Our results give an estimation of the size and spacing of a regular array of two dimensional islands aligned along the steps. Technologically, this is crucial to understand the spontaneous formation of quantum nanostructures. We compare our results to the results that Li et al [1] obtain via an energy minimization criteria. This work was partially supported by Conacyt under grant 33920-E and FENOMEC. We thank Hong Guo for having suggested us to look into this area.
[1] Adam Li, Feng Liu, D.Y. Petrovykh, J.-L. Lin, J. Viernow, F.J. Himpsel, and M.G. Lagally, Phys. Rev. Lett. 85, 5380 (2000).

2:30 PM N2.4/AA3.4
IMPROVING THE SIZE DISTRIBUTION OF InAs QUANTUM DOTS ON (100)InP. J. Lefebvre, P.J. Poole, J. Fraser, G.C. Aers, D. Chithrani, R.L. Williams, Institute for Microstructural Sciences, National Research Council, Ottawa, CANADA.

InAs self-assembled quantum dots on (100)InP are attractive because their emission wavelength is centered around 1.5 micron, and moreover their emission intensity depends only weakly on temperature up to 300K. However, this system suffers from the broad distribution of quantum dot size, which is attributed to a smaller lattice mismatch compared with the GaAs system, and to exchange processes between group V species. InAs self-assembled quantum dots have been grown

on InP nano-templates fabricated in-situ by chemical beam epitaxy. Electron microscopy on surface quantum dots and photoluminescence on buried quantum dots show a significant improvement of their uniformity. The result is due to spatial ordering of quantum dots.

3:15 PM *N2.5/AA3.5
SELF-ASSEMBLY OF NANOWIRES ON STEPPED SILICON: FROM ATOMIC CHAINS TO INTERCONNECTS. F.J. Himpsel, UW-Madison, Dept of Physics, Madison, WI.

One-dimensional objects, such as strings of atoms, organic molecules, nanodots, and nanowires can be produced on stepped silicon surfaces by self-assembly. Step decoration, strain-induced ordering, lattice match, and a match of the electronic states are among the driving forces. These structures can be used for studying electrons in one dimension, for memory arrays at the atomic limit, and as interconnects. For details see: http://uw.physics.wisc.edu/ himpsel/

3:45 PM N2.6/AA3.6
STRUCTURAL PROPERTIES IN SELF-ORGANIZED BURIED WIRES. Tomas Roch, Anke Hesse, Julian Stangl, Günther Bauer, Johannes Kepler University, Institute for Semiconductor Physics, Linz, AUSTRIA; Karl Brunner, Technical University, Walter-Schottky Institut München, GERMANY.

Self-organized quantum wires were created during heteroepitaxial growth of SiGe/Si multilayers. The multilayers have been deposited on a (001) Si substrate with 3.5 degree miscut. The multilayer consisted of 20 periods of $Si_{0.55}Ge_{0.45}$/Si (2.5nm/10nm)and it was capped by 12 nm Si. From TEM investigations, a periodic wire structure along [100] with a average wire distance of 90 nm is apparent. The shape of the buried wires and their mean chemical composition were studied by x-ray scattering. The wire morphology was determined using grazing-incidence small-angle x-ray scattering (GISAXS) which is insensitive to the deformation field induced due to the mismatch of the wire lattice with respect to the Si matrix. Contratry, the wide-angle scattering (grazing-incidence diffraction, GID) is influenced mainly by this deformation field. Therefore, combining these methods with elasticity simulations and using the well-known dependence of the mismatch on the Ge content, we were able to determine non-destructively both the wire shape and their average chemical composition. Using the wire shape obtained by GISAXS, we have simulated both the deformation field of a buried wire and the reciprocal space distribution of the x-ray intensity scattered in a GID experiment. Comparing this distribution with the experimental data we determined the mean Ge content in a buried wire to (50 ± 10)%. From the GID measurements, it also follows that the mean lateral elastic relaxation of the wire structure is rather small and it does not exceed $\epsilon_{xx} \approx 7 \times 10^{-4}$. The mechanism of the wire growth determines the shape of its cross-section. In this study, we have approximated the actual shape of the wire cross-section by a triangle, with its base parallel to the wetting layer. If the wires were created only by a bunching process of the monolayer steps present at the growing vicinal surface, the angle of the longer side of the triangular wire shape would not exceed the miscut angle. However, from the GISAXS we obtain a value of (6± 1)°. This indicates that the process of self-organization cannot be explained by step bunching alone, and another mechanism controlling the surface diffusion of the adatoms must be involved.

4:00 PM N2.7/AA3.7
SELF-ASSEMBLED LATERAL STRAINED QUANTUM WELLS IN MOVPE AlInAs ALLOYS. Andrew Norman, Sebastien Francoeur, Mark Hanna, Angelo Mascarenhas, Mowafak Al-Jassim, National Renewable Energy Laboratory, Golden, CO.

Self-assembled strained InAs-rich lateral quantum wells have been spontaneously formed by phase separation in AlInAs alloy layers grown by metal-organic vapor-phase epitaxy at low temperatures. InAs-rich wells of the order of 10 nm wide, over a micron long, and aligned along the [110] direction have been produced. The resulting structures exhibit a large band gap reduction and strongly polarized optical transitions. We will report how the microstructure and properties of these lateral quantum wells may be altered by growth on offcut (001) InP substrates and discuss possible growth mechanisms for these spontaneously formed nanostructures.

4:15 PM N2.8/AA3.8
SPONTANEOUS PATTERN FORMATION DURING ION BOMBARDMENT WITH AND WITHOUT TEMPLATES. Alexandre Cuenat, Michael J. Aziz, Harvard University, Division of Engineering and Applied Sciences, Cambridge, MA.

We study the formation and self-organization of ripples and dots spontaneously appearing during uniform irradiation of Si with energetic ion beams. Features have been produced both with sub-keV Argon ions and with a 30 keV Ga Focused Ion Beam (FIB). Spontaneously self-organized features have been observed at temperatures as low as room temperature. It appears that the edge of the sputtered region influences the patterns formed in this process and we will report on our efforts to guide the self organization by the imposition of lateral boundary conditions on the sputter instability. Comparison with other materials and possible mechanism for the formation of the ripples will be discussed.

4:30 PM N2.9/AA3.9
REAL SPACE ANALYSIS OF COLLOIDAL EPITAXY. Jacob P. Hoogenboom[a], Anja K. van Langen-Suurling[c], Hans Romijn[c], Alfons van Blaaderen[a,b], [a]FOM Inst AMOLF, Amsterdam, THE NETHERLANDS; [b]Utrecht University, Physics and Chemistry of Condensed Matter, Debye Inst, Utrecht, THE NETHERLANDS; [c]Technical University of Delft, DIMES, Delft, THE NETHERLANDS.

Using fluorescently labeled core-shell colloids and confocal microscopy structural and dynamical aspects of 3D crystallization can be studied quantitatively in real-space [1,2]. We performed various experiments using colloidal epitaxy to both grow large, well-oriented 3D-crystals and to study (epitaxial) crystallization [2]. We show that by using patterned substrates, any stacking sequence of hard-spheres can be grown, including a hexagonal close packed crystal that has a higher free energy than any other close-packed hard-sphere crystal structure. Furthermore, we studied the stability of these crystals upon lattice vector stretches in the pattern and we examined the structure and evolution of reconstructions and incommensurate crystals that grow beyond this stability range. Using optical tweezers we can locally manipulate the patterning of colloids on a substrate and study the effects of defects and small (irregular) grains in subsequent 3D crystal growth. Apart from hard-sphere systems under gravity, the effects of patterned walls on the crystallization behavior of charged, density-matched colloids were also investigated and compared to computer simulations [3]. A simple pattern of equally spaced, charged lines was found to induce (110) oriented face centered cubic crystals of charged particles. Colloidal Epitaxy provides not only a means to grow large, well-oriented 3D-crystals with characteristic spacings in the photonic range, but also allows fundamental study of epitaxial crystal growth quantitatively in 3D and in real space.
[1] W.K. Kegel, A. van Blaaderen, Science **287**, 290 (2000).
[2] A. van Blaaderen, R. Ruel, P. Wiltzius, Nature **385**, 321 (1997).
[3] M. Heni, H. Lowen, Phys. Rev. Lett. **85**, 3668 (2000).

4:45 PM N2.10/AA3.10
TIN AND SULFURS' EFFECTS ON THE Pb ON Cu(111) SELF-ASSEMBLING SYSTEM. Richard Plass, Gary L. Kellogg, Sandia National Laboratories, Albuquerque, NM.

As a follow up to the discovery of self-assembly in the Pb on Cu(111) surface (1), we have investigated the effects which sulfur and tin have on this system. The self-assembly of this system involves surface domain patterns of a Pb and Cu surface alloy with no long range order and an incommensurate Pb overlayer reconstruction. We find that very small amounts of sulfur, a common contaminant in Cu single crystals, significantly enhances the mobility of the surface domains. However fraction of a monolayer amounts of sulfur hinder surface mobility. In the tin case, the Cu(111)-($\sqrt{3}$x$\sqrt{3}$)R30° Sn surface alloy assumes the role of the Pb / Cu random surface alloy in the self assembly process and segregates from the lead, which remains in the overlayer phase. While the presence of tin slows down the Pb overlayer domains compared to the pure Pb case, self-assembling patterns still form. I will also discuss some properties of the Cu(111)-(4$\sqrt{3}$x4$\sqrt{3}$)R30° Pb Sn, Cu(100)-(5x4) Pb Sn, and Cu(100)-($\sqrt{50}$x$\sqrt{50}$)R8.1° Pb Sn reconstructions we have identified. 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. (1) R. Plass, J.A. Last, N.C. Bartelt, and G.L. Kellogg, Nature, accepted for publication.

SESSION N3: POSTER SESSION
Chairs: Eric H. Chason and Robert Hull
Monday Evening, November 26, 2001
8:00 PM
Exhibition Hall D (Hynes)

N3.1
ATOMISTIC SIMULATIONS OF DEPOSITION PROCESSES OF EPITAXIAL LAYERS. K. Shintani, H. Sugii, M. Nishimura, T. Nakajima, Univ of Electro-Communications, Dept of Mechanical Engineering and Intelligent Systems, Tokyo, JAPAN.

The deposition processes of epitaxial layers are simulated by the method of molecular dynamics. The interaction forces between atoms are calculated by using the Stillinger-Weber potential. Before the deposition of atoms, the substrate is equilibrated at a specified

temperature. The atoms with the identical initial velocities and with the somewhat different initial coordinates in the plane parallel to the growth surface arrive at the substrate to form an epitaxial layer. During the deposition, the lower part of the substrate is held at the initially specified temperature by velocity scaling. The growth morphology of an overlayer is dependent on the initial velocities of deposited atoms and on the substrate temperature. How the growth morphology is influenced by such parameters is investigated in connection with the behaviors of deposited atoms.

N3.2
ON THE APPLICABILITY OF THE RATE EQUATION MODEL FOR THE DESCRIPTION OF LAYERED EPITAXIAL GROWTH KINETICS IN THE PRESENCE OF AN EHRLICH-SCHWOEBEL BARRIER. Vladimir Trofimov, Vladimir Mokerov, Inst of Radioengr & Elec of RAS, Dept of Nanoelectronics, Moscow, RUSSIA.

In the past decade, much theoretical efforts have been devoted to a deeper understanding of layered epitaxial growth in the presence of an Ehrlich-Schwoebel (ES) barrier at an island edge. To that end a number of models for nucleation on top of a growing island with taking into account the presence of an ES barrier, based on the rate equation approach, have been developed. These models discovered smooth/rough growth transitions induced by repulsive ES barrier and corresponding phase diagrams of the growth mode in the parameter space have been constructed and it has been shown that models predictions are in a reasonable agreement with the available experimental data. However, in just recently published articles results of kinetic Monte Carlo simulations that substantially disagree with rate equation model predictions have been reported and remarked that the applicability of mean field rate equations to the confined geometry on an island atop is not obvious, and an alternative theory based on a concept of a residence time of an adatom on top of an island has been proposed. In this paper, we present a more careful analysis of the rate equation-based models in view of these novel results and critical comments. This analysis shows that despite the spatial limitations of the rate equation-based models they are valid at least in the case of not very small islands (i.e., not very strong barrier) where the most interesting growth mode transition phenomena are developed.

N3.3
PLASTIC EFFECTS ON THE FRONT INSTABILITY CAUSED BY A UNI-AXIAL STRESS: A PHASE-FIELD APPROACH. Patrick Berger, Chaouqi Misbah, Klauss Kassner, GREPHE, LSP, Univ. J. Fourier, Grenoble, FRANCE.

The description of growth processes with the phase-field approach, consists in representing the transition zone between the two coexisting phases by the gradual change of this field from its value in one phase to its value in the other one. Such a method has been recently applied to the study of the Asaro-Tiller-Grinfeld (ATG) instability which manifests itself as a surface corrugation of an uniaxially stressed solid in contact with its melt (Kassner et al. Phys. Rev. E 63, 036117 (2001)) or with vacuum. Analytical and experimental results have been recovered and further investigations show that the periodic array of grooves obtained at early stage generically evolve into a superstructure which arises from a serie of imperfect period doublings. This coarsening process does not seem to stop and implies a great accumulation of stress in the grooves. We study the effect of stress release by plastic deformation and analyze coarsening (if any) and the possible transition to a selected steady-state periodic structure.

N3.4
ATTRACTIVE STEP INTERACTIONS ON VICINAL Si(113) SURFACES. Cristian V. Ciobanu and Vivek B. Shenoy, Division of Engineering, Brown University, Providence, RI.

Experimental studies on vicinal Si(113) have shown that the steps on this surface tend to self-organize in bunches depending on temperature and vicinal angle. Such step-bunched surfaces are of considerable technological relevance as they can serve as templates for growing quantum dots and wires. A model hamiltonian for the interacting steps, that captures the physics of step bunching and the transitions between different bunches has recently been proposed by Shenoy *et. al* in PRL **81** (1998) and Surf. Sci. **467** (2000). This model includes both the long range repulsive interactions between the steps due to elastic effects as well as a short-range attractive interaction. We have carried out atomic-scale studies of step-step interactions for several different surface reconstructions of the Si(113) surface in order to determine the magnitudes of the repulsive and attractive step interactions. Our results are compared with experimentally determined interaction parameters of Sudoh *et. al* (Surf. Sci. Lett.**452**, 2000) and Yoon *et. al.* (Surf. Sci. **411**, 1998).

N3.5
LOW LEVEL Si ALLOYING IN Ge/Si(001) ISLANDING: ELEMENTAL CONTENT AND STRUCTURE. Anat Eshed, Univ. of Texas at Arlington, Physics Dept., TX; Jinggang Zhu, Jiong Yan, Univ. of Texas at Arlington, Materials Science and Engineering Dept, TX; Robert Beserman, Technion, Israel, Physics Dept., ISRAEL; Alex Weiss, Univ. of Texas at Arlington, Physics Dept, TX.

We have investigated the shapes, thickness, density, composition, and quality of Ge/Si(001) islands grown by solid source molecular beam epitaxy in ultra high vacuum conditions. Nano crystals were formed by means of the Stranski-Krastanov self assembled growth mechanism. 5 nm of Ge was deposited on Si(001) substrates, at 500°C, with deposition rate of 0.5 nm/min. Atomic force microscope measurements reveal islands of mainly three types, in which the smallest has been classified as square based huts or pyramids, with 30 nm average height and diameter of about 60 nm. In addition two types of clusters were found: one composed of two islands, prism shaped, with triangle cross section from one direction (90 nm base), and rectangular cross section from the perpendicular direction (140 nm long) with average height 35 nm. The largest type of islands found consists of four adjacent islands. Typical sizes for those islands are 700 nm in diameter and 80 nm in height. Islands density found to be correlated with their sizes, with denser areas containing mostly islands of the smaller sizes. Micro Raman spectroscopy, with probing spot of about 0.7 micron diameter, has been used to study the composition, thickness and crystalline quality of the islands. Data were taken at various points on the sample distinguishing between various islands types. Combined analysis of Raman spectra and the micrographs reveal low amount of alloying (less than 30%) in all types of islands, with the larger islands showing the more amount of intermixing. High crystalline quality of the layers within the islands suggests negligible amount of dislocations.

N3.6
INTERDIFFUSION AT SILICON / ALUMINUM INTERFACES. Karla Balzuweit, LBNL, National Center for Electron Microscopy, Berkeley, CA and UFMG, Departamento de Fisica, Belo Horizonte, BRASIL; Ulrich Dahmen, LBNL, National Center for Electron Microscopy, Berkeley, CA.

The importance of aluminum films on silicon substrates is well known, especially in the semiconductor industry. Aluminum films remain a very important material for metallization in silicon integrated circuits. Although it is well-known that aluminum spike formation at the interface leading sometimes to device failure, the exact mechanisms causing this type of failure, and the underlying mechanism of interdiffusion are still not well understood. Previous studies in the Al-Si system [Thangaraj et al. (1992a), Thangaraj et al. (1992b), Thangaraj et al. (1994), Westmacott et al. (in press)] showed some differences in the film structure depending on the crystallographic orientation of the substrate. Aluminum films, with various thicknesses were grown by physical vapor deposition on both silicon (100) and (111). On Si (100) substrates held at 280°C, Al formed (110) bicrystal structures where the two variants are related by a 90° rotation. On Si (111) substrates, either a polycrystalline film, a (001) tricrystal film structure, or a (111) single crystal structure can be obtained at different deposition temperatures. These different film orientations are characterized by different interface structures, which in turn are shown to be related to the mechanism of interdiffusion during heating. To investigate these processes, in-situ and ex-situ heating experiments including thermal cycling were carried out in scanning and transmission electron microscopes. During heating, Si dissolution in the Al film depended on the substrate orientation. During cooling, Si reprecipitated mainly at the film surface. The mechanism of interdiffusion and the crystallographic and morphological character of spikes and precipitates were characterized in detail by electron microscopy. N. Thangaraj, K.H. Westmacott and U. Dahmen Appl. Phys. Lett. 61 (1) 1992 - 37-39 N. Thangaraj, K.H. Westmacott and U. Dahmen Appl. Phys. Lett. 61 (1) 1992 - 913-915 N. Thangaraj, S. Hinderberger, K.H. Westmacott and U. Dahmen Conference Proceedings ULSI-XI 1994 Materials Research Society.

N3.7
LATERAL COMPOSITION MODULATION IN MIXED ANION COMPOUND SEMICONDUCTOR STRUCTURES. Catalina Dorin and Joanna Mirecki Millunchick, Department of MS&E, University of Michigan, Ann Arbor, MI.

In this work, we demonstrate for the first time lateral composition modulation (CM) in GaAs/GaSb short period superlattices (SPS). Several different structures were investigated in order to study the role of Group V overpressure on the final composition and uniformity of the structure. It was found that for lattice matched SPS (As:Sb ratio 10:1) the layers are intermixed and there is no lateral CM. Adding a growth interruption between the individual SPS layers causes more As incorporation into the films. When the As:Sb ratio was 2:1, CM was observed. For example, the X-ray Diffraction (XRD) Reciprocal Space Maps show that the SPS consisting of 2 MLs of both GaAs and GaSb have diffuse lateral satellites, indicative of composition modulation. Cross Section Transmission Electron Microscopy (XTEM)

micrographs reveal that the film is indeed phase separated, however, it is extremely irregular. This is not unexpected considering that the Reflection High Energy Electron Diffraction (RHEED) pattern showed that faceted islands were present on the surface during growth. For an SPS consisting of 1 ML of GaAs and 2 MLs of GaSb, the XRD Reciprocal Space Maps show stronger lateral satellites. XTEM images corroborate the presence of relatively regular lateral CM in this sample. The CM observed in these films is a result of the SPS growth and not due to spinodal decomposition, as evidenced by the fact that an alloy grown at the same conditions results in a homogeneous film. These results suggest that some residual roughness is required for lateral CM to occur, however, too much roughening destroys the lateral periodicity. Furthermore, we will show that surface segregation contributes to the formation of lateral CM.

N3.8
A NEW SPONTANEOUS ORDER IN LATTICE-MISMATCHED INTERFACES: BINARY SUPERLATTICE OF GRAINS IN Si/Si_3N_4 NANOPIXELS. Elefterios Lidorikis, Rajiv K. Kalia, Aiichiro Nakano, and Priya Vashishta, Concurrent Computing Laboratory for Materials Simulations and Biological Computation and Visualization Center, Dept of Physics & Astronomy and Dept of Computer Science, Louisiana State Univ, Baton Rouge, LA; Martina E. Bachlechner, Dept of Physics, West Virginia Univ, Morgantown, WV.

We use a hybrid atomistic/continuum simulation approach to study the strain relaxation mechanisms in lattice-mismatched Si/Si_3N_4 nanopixels. The elastic strain energy of the mismatched system is relaxed through the formation of line interfacial defects similar to misfit dislocations. These line defects are the result of successive slips of the interface between two nearly-degenerate interface equilibrium configurations C1 and C2. These slips are along the Si $< -2, 1, 1 >$ directions and the corresponding grain boundaries in the Si $< -1, 0, 1 >$ directions. This strain relaxation mechanism results in a triangular network of interfacial line defects that frames a triangular binary superlattice of grains C1 and C2. High stresses appear at the vertices where the grain boundaries meet. Work supported by AFOSR, NSF, DOE, NASA, DoD-DURINT and BCVC (Louisiana Board of Regents). Simulations were performed on parallel machines at the CCLMS.

N3.9
CARRIER REDISTRIBUTION IN SELF ASSEMBLED InAs/InP QUANTUM WIRES. Hyosin Choe, P.W. Yu, Dept of Information and Communications, Kwangju Institute of Science and Technology (K-JIST), Kwangju, KOREA; Haeyeon Yang, Gregory J. Salamo, Dept of Physics, University of Arkansas, Fayetteville, AR; J.S. Yim, Y.D. Jang, U.H. Lee and D. Lee, Dept of Physics, Chungnam National Univ, Taejon, KOREA.

We have studied the photoluminescence (PL) and time-resolved photoluminescence (TRPL) of self assembled InAs quantum wires (QWRs) grown by molecular beam epitaxy on an InP (001) surface. Two emission peaks positioned at 1.05 eV (peak A) and 1.01 eV (peak B) were observed in PL measured at 8 K and the intensities of both peak increase linearly with increase in the excitation power. In temperature dependent PL measurement ranging from 8 to 300 K, the ratio of peak B to peak A in integrated PL increases continually with increase in temperature. As temperature increases from 8 to 300 K, the decay times of both peaks decrease from 1.37 ns and 1.53 ns to 0.88 ns and 0.85 ns for peak A and peak B, respectively. The decay of peak A is faster than that of peak B at 8 K but slightly slower than that of peak B at room temperature. The variation of PL intensity and decay time with temperature are attributed to effect of carrier density change in each energy state, i.e. carriers are redistributed by thermal energy due to hopping from peak A state to peak B state. The results obtained from excitation power and temperature dependence of PL indicate that both peaks are correspond to ground state of two different types of QWRs.

N3.10
OPTICAL AND STRUCTURAL PROPERTIES OF InAs EPILAYER ON GRADED InGaAs. Gu Hyun Kim, Jung Bum Choi, Chungbuk National Univ, Dept of Physics, Chungju, KOREA; Jae-Young Leem, Joo In Lee, Sam Kyu Noh, Jong Su Kim, Jin Soo Kim, Se-Kyung Kang, Korea Research Institute of Standards and Science (KRISS), Materials Evaluation Center, Taejon, KOREA.

We have studied infrared photoluminescence (PL), transmission electron microscopy (TEM) and x-ray diffraction (XRD) of 400 nm and 1500 nm thick InAs epilayers directly grown on GaAs, and 4 nm thick InAs on graded InGaAs layer with total thickness of 300 nm by molecular beam epitaxy. The PL peak position of 400 nm, 1500 nm and 4 nm InAs epilayer measured at 10 K are blue shifted from that of InAs epilayer on InAs substrate by 6.5, 4.5, and 6 meV, respectively, which could be mainly explained by the residual strain in the epitaxy. The residual strain caused by the lattice mismatch between InAs and GaAs or graded InGaAs/GaAs was observed from XRD measurements. While the PL peak position of 400 nm thick InAs layer is linearly shifted toward higher energy with increase in excitation intensity ranging from 10 to 140 mW, those of 4 nm InAs epilayer on InGaAs and 1500 nm InAs layer on GaAs is gradually blue-shifted and then, saturated above a power of 75 mW. From the results, adopting graded InGaAs layer between InAs and GaAs could more efficiently reduce the strain due to lattice mismatch in the structure of InAs/GaAs.

N3.11
OPTICAL AND STRUCTURAL PROPERTIES OF HEIGHT-CONTROLLED InAs QUANTUM DOTS. Jin Soo Kim, Phil Won Yu, Kwangju Institute of Science and Technology (K-JIST), Dept of Information and Communications, Kwangju, KOREA; Jae-Young Leem, Joo In Lee, Sam Kyu Noh, Jong Su Kim, Gu Hyun Kim, Se-Kyung Kang, Korea Research Institute of Standards and Science (KRISS), Materials Evaluation Center, Taejon, KOREA; Yu Dong Jang, Uk Hyun Lee, Jung Soon Yim, Donghan Lee, Chungnam National Univ, Dept of Physics, Taejon, KOREA.

The optical and structural properties of height-controlled InAs quantum dots (QDs) have been investigated by photoluminescence (PL) and transmission electron microscopy (TEM). By depositing 1.4 nm $In_{0.08}Ga_{0.92}As$ and 0.8 monolayer (ML) InAs layer with different periods on 2 ML InAs QDs, the height of InAs QDs was systematically controlled with same lateral size. The PL peak position is shifted toward longer wavelength with increase in the aspect ratio (height/width) of QDs as observed from TEM measurements. The PL peak position of InAs QDs with the highest ratio is 1.27 μm with PL linewidth broadening of 30 meV at room temperature. As the aspect ratio is increased, the full width at half maximum (FWHM) in PL measured at 10 K is decreased from 86 meV to 33 meV indicating that the inhomogeneous broadening caused by the fluctuation in QD height is reduced. With increase in the aspect ratio, the change in peak position and FWHM is less sensitive to the height. In TEM image, there is also no significant misfit dislocation caused by strain relaxation, which can be easily seen in the large QDs.

N3.12
Abstract Withdrawn.

N3.13
UHV-STM STUDY OF ION-ASSISTED GROWTH OF Ge ON Si SURFACES. J. Matsuo, T. Seki T. Aoki and G.H. Takaoka, Ion Beam Engineering Experimental Laboratory, Kyoto University Sakyo, Kyoto, JAPAN.

Ion assisted deposition technique is widely used for high quality film formation. However, the role of ion bombardment during film growth is not well understood. Ultra High Vacuum Scanning Tunneling Microscope (UHV-STM) system has been used to examine ion bombardment effects and nucleation growth at various temperatures. Single ion impact traces whose diameters were about 20A were clearly observed with atomic resolution on the Si(111) 7 Å $\sim$7 surface irradiated with 500eV Xe ions at 400°C. The vacancies created in sub-surface by the ion impact diffuse toward the surface and form vacancy clusters on the surface. These vacancy clusters play a very important role in Ge films growth. Many small Ge islands was observed on the surfaces deposited a few A of Ge atoms at 400°C. Vacancy clusters become nucleation site of Ge islands. However, deposited Ge atoms diffuse and coalesce into step edges on the unirradiated surfaces at this temperature. We also examined nucleation process of Ge atoms during high temperature annealing. Ge atoms were deposited both clean and Xe irradiated surface at room temperature. Large Ge islands, whose diameter was a few tens of nm, are formed on the clean surface after annealing at 600°C. Small Ge islands connected each other like a network were found on the ion irradiated surface. Growth kinetics modified with ion irradiation will be discussed.

N3.14
STM ANALYSIS OF COPPER THIN FILMS USING HYPERTHERMAL COPPER IONS. Joshua M. Pomeroy, B.H. Cooper, Joel D. Brock, Cornell Center for Materials Research (CCMR), Cornell University, Ithaca, NY.

STM analysis of thin copper films grown on Cu(111) at room temperature using hyperthermal ions reveals several morphological features not present in thermally grown films. Hyperthermal deposition of thin films has become a popular industrial technique due to observed decreases in film roughness and stress with increased grain sizes, but the link between incidence energy and these properties is poorly understood. Using a sophisticated molecular dynamics (MD) and kinetic Monte Carlo molecular dynamics hybrid simulation (KMC-MD), surface structures observed in experimentally grown films are correlated with the activation of athermal atomistic

mechanisms in the MD. Strong evidence will be presented for the activation of adatom/vacancy formation near 20 eV, and for the activation of step-enhanced sputter erosion near 60 eV. Mechanisms beneficial for smooth growth, such as atomic insertion near 10eV, have been proposed but are more difficult to correlate with the data due to their subtle morphological signatures.

N3.15
GaAs HETEROEPITAXY ON FLUORIDE BY ELECTRON BEAM INDUCED SURFACE MODIFICATION. T. Fritz, M. Haiml, S. Schön, U. Keller, Swiss Federal Institute of Technology Zurich, SWITZERLAND.

Semiconductor saturable absorber mirrors (SESAMs) are devices for ultrashort pulse generation, which combine the nonlinear optical properties of a semiconductor saturable absorber with those of a high reflection mirror in one device. The performance of a SESAM device is measured in terms of nonsaturable losses. These losses can be caused by scattered light, which originates from device interfaces and surface. In particular post-growth processing as applied for conventional SESAMs based on silver mirrors degrades the surface and introduces nonsaturable losses due to scattered light. Therefore, we have introduced a novel monolithic ultrabroadband AlGaAs/CaF_2 SESAM for the generation of sub-10 fs laser pulses. Since CaF_2 has a very low surface energy the growth of the GaAs saturable absorber layer produces rough surfaces due to island growth. An rms roughness of up to 20 nm and scatter losses of up to 6% have been measured. In order to study the nucleation of the GaAs on the CaF_2, the fluoride surface is exposed to an electron beam of different doses using high electron energies of up to 20 keV and thermal electrons before and during growth. Due to electron exposure the CaF_2 surface deteriorates by evaporating fluorine. The surface free energy is increased. AFM analysis and scattered light experiments demonstrated a rms surface roughness of 10 nm and scattered light of 0.7% for the highest electron energy applied. Therefore, the monolythical grown GaAs/CaF_2 multilayer stack is already competitive to a silver mirror based SESAM with scattered light losses of 0.5% at the lowest. However, less losses due to scattered light are obtained by exposing the fluoride surface to thermal electrons. The amount of scattered light was reduced to 0.06%. The decrease by one order of magnitude is not only due to the small reduction in surface roughness, but also caused by a change in the shape of the islands.

N3.16
CHARACTER OF DEFECTS AT AN ION IRRADIATED BURIED THIN-FILM INTERFACE. Ramki Kalyanaraman, Oak Ridge National Laboratory, Oak Ridge, TN and Agere Systems, Murray Hill, NJ; Tony Haynes, Wayne Holland, Oak Ridge National Laboratory, Oak Ridge, TN; George Gilmer, Agere Systems, Murray Hill, NJ.

The integration of different materials to create devices on a single chip with multiple functions involving optical, electrical and mechanical interactions is presently a rapidly growing field of interest. The various interfaces and differences in properties such as thermal expansion impose important complications in achieving the required materials integration. Ion implantation provides the capability to fine-tune the properties of these integrated structures due to its ability to deposit energy and matter at appropriate positions. In this regard, the consequence of implantation through various interfaces must be understood. In this work, we have studied the effect of ion implantation through a c-Si/SiO_2/c-Si heterostructure. We have performed high-energy ion implantation into such a structure having a 0.2 μm thick SiO_2 layer at a depth of 1.5 μm. Using a recently developed technique, Au labeling, we show that besides the expected excess vacancy (V^{ex}) defects in the Si overlayer an additional defect peak occurs at the front side of the buried Si/SiO_2 interface. By injecting additional Si atoms into this region, we determined the defects to be vacancy-type in nature. We have quantitatively studied the interface V^{ex} concentration as a function of Si ion dose. The presence of this V^{ex} peak near the interface is also predicted by the binary collision code TRIM and is related to a discontinuity in the flux of recoiled atoms due to the presence of the Si/SiO_2 interface. Further, we also show using TRIM that the nature of the defects at the interface can be changed from vacancy to interstitial-type by adjusting certain physical characteristics of the buried thin film, such as its density and the atomic masses of its constituents. This result suggests the possibility of using ion beams to selectively modify the strain near interfaces during and after heteroepitaxial growth.

N3.17
STRAIN RELAXATION OF HE^+ IMPLANTED, PSEUDOMORPHIC $Si_{1-x}Ge_x$ LAYERS ON Si(100). B. Hollander, S. Mantl, St. Lenk, H. Trinkaus, D. Kirch, M. Luysberg, ISG/IFF Forschungszentrum Jülich GmbH, Jülich, GERMANY; Th. Hackbarth, H.-J. Herzog, DaimlerChrysler Forschungszentrum Ulm, Ulm, GERMANY; P.F.P. Fichtner, Dept. de Metalurgia, UFRGS, Porto Alegre, BRAZIL.

Strain relaxed $Si_{1-x}Ge_x$ layers on Si(100) allow the growth of Si quantum well layers under biaxial tensile strain which is required to obtain a sufficiently large conduction band offset for the formation of a two dimensional, high mobility electron gas. We report on the strain relaxation of initially pseudomorphic $Si_{1-x}Ge_x$ layers (x=0.1 ... 0.45) grown by molecular beam epitaxy on Si(100) after subsequent helium ion implantation and annealing. Implantation was performed with energies between 5 keV and 30 keV and doses between 1 x 10^{16} cm^{-2} and 3 x 10^{16} cm^{-2} in order to produce nanocavities slightly below the interface during annealing. The samples were investigated by Rutherford backscattering and ion channeling. X-ray diffraction and transmission electron microscopy. Residual strain and threading dislocation density will be discussed as a function of implantation dose and thermal treatment. First measurements of electron mobility in QW- and MODFET-structures grown on these relaxed layers showed excellent results comparable to structures grown on well established, thick, graded $Si_{1-x}Ge_x$ buffer layers. A model for the implantation induced strain relaxation mechanism is proposed, which assumes the formation of short misfit dislocation segments form dislocation loops punched out by gas filled nanocracks.

N3.18
TEMPERATURE-DEPENDENT STRAIN RELAXATION BEHAVIOR OF InGaAs/GaAs INVESTIGATED BY IN SITU MONITORING. C. Lynch, E. Chason, R. Beresford, D.C. Paine, E.B. Chen, K. Tetz, Brown University, Division of Engineering, Providence, RI.

In situ stress monitoring has been used to measure the kinetics of stress relaxation during MBE growth of strained thin films of $In_xGa_{1-x}As$/GaAs. This technique has allowed the real-time relaxation behavior of this system to be studied under various growth conditions. Beyond the Matthews-Blakeslee critical thickness, we observe two mechanisms that significantly relax the stress. The first mechanism is temperature-dependent and becomes active at a lower thickness as the temperature is increased. The second relaxation mechanism is independent of temperature over the measured range (450°C to 550°C) and relaxes significantly more stress than the first mechanism. Monitoring the stress during pauses in growth (with and without changing temperature) has shown that the relaxation behavior is kinetically limited during the early stages of growth. We relate these features of the relaxation evolution to misfit dislocation formation and multiplication and to the surface morphology.

N3.19
STRESS GENERATION AND RELAXATION DURING FILM HETEROEPITAXY ON A COMPLIANT SUBSTRATE WITH A VISCOELASTIC GLASS INTERLAYER. Zhaohua Feng, Edward G. Lovell, Roxann L. Engelstad, University of Wisconsin, Computational Mechanics Center, Mechanical Engineering Department, Madison, WI; Thomas F. Kuech, Peter D. Moran, University of Wisconsin, Chemical Engineering Department, Madison, WI.

Large stresses caused by the lattice mismatch between the film and substrate during heteroepitaxial growth lead to high dislocation densities in the film, which adversely affect the film quality and characteristics. Compliant substrates are an approach to reduce these stresses during growth by significantly reducing the stiffness of the substrate, decreasing the stresses and hence prevent dislocation development in the film. The compliant substrate discussed in this paper consists of three layers: a thin template, a mechanical handle wafer and a borosilicate glass interlayer bonding the template to the handle wafer. It is very difficult to directly measure film stresses in real time during its use within a growth system. Thus, finite element models were developed to analyze the complete stress and strain fields. The film and substrate were modeled as a multilayer shell system, with compatibility conditions imposed between layers. The materials of the film and template were purely elastic, whereas the borosilicate glass at the film growth temperature was viscoelastic. Transient simulation techniques were applied to analyze the system continuously and provide all stress components throughout the film and template at any stage of the growth process. The viscosity of the borosilicate glass had a significant influence on the stresses. Increasing the boron oxide content of the glass lowered the viscosity and accelerated the relaxation. Effects of radius, thickness and mismatch strains on the stress generation and relaxation were also established. The models clearly illustrate the influence of substrate compliance unique to a viscoelastic glass interlayer. Such simulations can be used to optimize process parameters of film growth and facilitate the design of new compliant substrate systems.

N3.20
STRESS ORIGIN AND RELAXATION IN EPITAXIAL AlN THIN FILMS ON SiC. Ravi Bathe, R.D. Vispute, R.P. Sharma, T. Venkatesan, CSR, Dept of Physics, Univ of Maryland, College Park, MD; C.J. Scozzie, Ken Jones, ARL, Adelphi, MD.

Heteroepitaxially grown AlN thin films on SiC have a tremendous potential towards high temperature and high power electronics. Due to a wide band gap (6.2eV), high thermal stability, and small lattice mismatch to SiC (1%), epitaxally grown AlN thin films seem to be promising candidates for dielectric applications and ion-implantation anneal cap. We have investigated the epitaxy, interfaces, surfaces and defects in epitaxial AlN thin films grown on SiC by pulsed laser deposition. In this paper, we report on the stress origin, evolution, and relaxation in heteroepitaxial AlN films grown on SiC. The crystalline structure and surface morphology of the epitaxially grown AlN thin films on SiC (0001) substrates have been studied using x-ray diffraction (θ-2θ, ω, and ϕ scans) and atomic force microscopy, respectively. The defect density and analysis have been studied by using Rutherford backscattering spectrometry, ion channeling technique and transmission electron microscopy. The films were grown at various substrate temperatures ranging from 500°C to 1100°C. X-ray diffraction measurements show highly oriented AlN films above growth temperature of 750°C, and single crystalline nature above 800°C. The films grown in the temperature range of 950°C to 1000°C have been found to be highly strained, where as the films grown above 1000°C were found to be relaxed after crack propagation along the crystallographic axes. The results on stress as a function of growth temperature, defects induced in the heteroepitaxial systems, thermal mismatch, growth mode, and buffer layers affecting the stress levels in the films will be presented, and the implication of these results for wide band gap power electronics will be discussed.

N3.21
COMPOSITION AND STRUCTURE OF EPITAXIAL CaF_2 LAYERS AT THE FIRST STAGES OF THEIR GROWTH ON Si(111). R. Würz, W. Bohne, W. Fuhs, J. Röhrich, M. Schmidt, A. Schöpke, and B. Selle, Hahn-Meitner-Institut, Silizium-Photovoltaik and Ionenstrahl-Labor, Berlin, GERMANY.

Thin epitaxial CaF_2 films when introduced as a buffer of a few monolayers were recently reported to modify the band offsets at the interface of heterojunction structures with Si. This would offer a promising approach to optimize the interface properties of Si-based heterojunction devices, for example of photovoltaic structures. We have grown CaF_2 films with thicknesses between 1 and 100 nm on Si(111) by evaporation from a CaF_2 source at UHV conditions. Because film composition and growth morphology near the interface with Si are supposed mainly to influence the bonding dipole configuration and, hence, the junction behavior, we have studied these properties by various techniques such as Heavy-Ion Elastic Recoil Detection Analysis (HI-ERDA), RBS/Channeling, X-ray Photoelectron Spectroscopy (XPS), Atomic Force Microscopy (AFM) and Auger Electron Spectroscopy (AES). The results of the surface sensitive XPS method could be calibrated by the RBS and HI-ERDA data which provide the element concentrations in absolute units. - Morphology and composition of the CaF_2 films strongly depend on the substrate temperature during the deposition. Epitaxial growth is observed at deposition temperatures above 450°C. The F/Ca ratio of the films in the monolayer range was found to deviate appreciably from the stoichiometric composition (F/Ca=2) suggesting that the interface composition does not obey the rules of bulk equilibrium chemistry. A principal-component analysis of the AES spectra shows the formation of different bonding configurations (including silicide-like bonds) at the CaF_2/Si interface. In order to get a two-dimensional film growth with minimum density of pin-holes we propose a template growth at two temperatures. First the substrate is covered by a complete CaF layer at 650°C at a rate of about 0.01 Å/s. The further growth is then accomplished with a higher rate (0.1 Å/s) at 500°C.

N3.22
IN SITU ANALYSIS OF OXIDE-ON-SILICON HETEROEPITAXY BY COAXIAL IMPACT-COLLISION ION SCATTERING SPECTROSCOPY. A. Sasaki, H. Isa, J. Tashiro, K. Nakajima, M. Yoshimoto, Tokyo Inst. of Tech., Yokohama, JAPAN; P. Ahmet, T. Chikyow, Nanomaterial Lab.-COMET, Tsukuba, JAPAN.

Heteroepitaxy for several oxide ultra-thin films on Si substrates were in situ examined by combined use of a coaxial impact-collision ion scattering spectroscopy (CAICISS) and the laser molecular beam epitaxy (laser MBE). CAICISS is a powerful tool to analyze oxide thin films' crystal structures, compositions and topmost surface atoms. By using CAICISS, it is able to obtain the atomic-scale information about the initial growth mechanism of oxide ultra-thin films on silicon substrates in real space. Cubic fluorite CeO_2 having an excellent lattice matching with Si is expected to be one of the most promising buffer layers that combine the silicon and various oxides exhibiting superior properties such as high-Tc superconductivity or ferroelectricity. Here, the low-temperature heteroepitaxial growth of CeO_2 films was investigated with focused on the in-plane epitaxial growth orientation. From in situ CAICISS measurements of the azimuth angle dependence of signal intensity, the type-B epitaxial growth ([-110]CeO_2||[1-10]Si) was verified for the films thicker than about 1 nm. It was confirmed that the initial growth mode can be determined by using CAICISS as a diagnostic tool during fabrication of ultra-thin films.

N3.23
EPITAXIAL GROWTH OF SELF-SIMILAR NANOMETER-SIZED Ag CIRCULAR DOTS ON H-TERMINATED Si(111) SURFACES. B.Q. Li, J.M. Zuo, University of Illinois, Department of Materials Science and Engineering and Materials Research Laboratory, Urbana, IL.

Epitaxial growth of nanometer-sized metallic dots and wires on semiconductors is an important step in the fabrication of atomic and molecular scale devices. One promising approach relies on the passivation of reactive surfaces and rendering of nano-structures on these chemically inert surfaces through self-organization. Understanding how atoms and molecules interact on these surfaces is key to effect the symmetry, dimensionality and morphology of the subsequent growth, and thus properties of the resulting nano-structures. With this motivation, we have investigated the growth of Ag nanoclusters on hydrogen passivated Si (111) surfaces compared using in-situ and ex-situ transmission electron microscopy characterization, XPS and AFM. The experiments show that the growth of Ag on hydrogen-terminated Si (111) surfaces is very different from that of bare Si surfaces. At room temperature deposition below 10 ML (monolayer) coverage, Ag grows with on hydrogen-terminated Si (111) surfaces in the form of dots with well-defined shapes and sizes. To understand this, we carried out systematic characterization of the size and shape distribution of Ag dots and the surface structure of passivated surfaces. XPS and AFM confirm chemically clean and flat surfaces. At room temperature, we find that at low coverage both triangle and irregular shaped Ag clusters exist. With the increase in coverage, cluster shape transforms from mostly pyramidal shapes to hexagonal and round mound shapes. The cluster dimension increases with coverage. The cluster size follows closely the distribution predicted by Ostwald ripening except at 10 ML coverage where initial coalescence is observed. The clusters are epitaxial with Ag(111)||Si(111). We observed a coverage dependent azimuthal alignment of 3-D clusters with a distribution of ~12° between 2 to 8 ML coverage. Comparison between experimental and simulated radial distribution of dots shows that the dots are randomly distributed with a well-defined diffusion exclusion zone.

N3.24
GROWTH OF TEXTURED Co FILM ON BURIED ULTRATHIN AMORPHOUS INTERLAYER MEDIATED BY Zr. D.K. Sarkar, INRS-Materials and Energy, University of Quebec, Varennes, Quebec, CANADA; M. Falke, G. Beddies, H. J. Hinneberg, Chemnitz University of Technology, Chemnitz, GERMANY.

Thin metals films of Zr of a thickness 0.5 nm to 10 nm were deposited on the chemically clean Si(100) substrates at room temperature using the magnetron sputtering method. A thin Co film of thickness 20 nm was deposited on the Si(100) substrates and on the top of Zr films without breaking the High Vacuum (HV). X-ray diffraction (XRD) and transmission electron microscopy (TEM) shows the highly textured Co film on Zr thin film substrates but not on Si(100) substrates. X-ray reflectivity and Cross-sectional transmission electron microscopy (XTEM) shows the presence of a buried amorphous interlayer between Co/Zr interface but not in Co/Si(100) interface. The results has been discussed on the basis of local temperature rise due to the amorphous phase formation and hence better mobility of the further deposited metal atoms which is the cause of highly textured Co thin films on Zr film substrates.

N3.25
EFFECTS OF MISFIT STRAIN ON PROPERTIES OF ZnO FILMS GROWN BY PULSED LASER DEPOSITION. M.C. Park, W.H. Yoon, D.H. Lee, J.M. Myoung, Yonsei University, Dept of Metallurgical Engineering, Seoul, KOREA; S.H. Bae, S.Y. Lee, I. Yun, Yonsei University, Dept of Electrical Engineering, Seoul, KOREA.

ZnO is a very attractive material for application to the optical devices such as blue-, violet-, and UV-light emitting diodes (LED_s) and laser diodes (LD_s), since it has a direct and wide band gap of 3.3 eV at room temperature. Moreover, owing to the large exciton binding energy of ~60 meV, ZnO thin films exhibit very strong emissions by excitons even at room temperature. In this paper, we report on the effect of the strain on the properties of ZnO thin films grown by pulsed laser deposition (PLD). A series of ZnO thin films having different thicknesses were prepared on c-plane sapphire substrate. After deposition, their structural, electrical, and optical properties were examined by DC-XRD, Hall, and PL measurements, respectively. It is found that, as the film thickness increases, the crystalline quality and the electrical properties of ZnO films are improved and, for the films thicker than 4000 Å, the misfit strain is almost relaxed. It is also

observed that, as the film thickness increases, the intensity of the band-edge emission increases. One interesting observation is the variation in positions of band-edge emission peaks- it changes from 3.23 eV for the 400-Å-thick film to 3.27 eV for the films thicker than 4000 Å. It is, therefore, concluded that, for the films thicker than 4000 Å, the strain due to the lattice mismatch between the film and the substrate is almost relaxed and the bulk ZnO properties are observed.

N3.26
STM CHARACTERIZATION AND MODELING OF Pt NANOCLUSTERS ON ANATASE TiO_2 (001) SURFACE.
Anter El-Azab, Pacific Northwest National Laboratory; Shupan Gan, Trilink Corp., CA; Yong Liang, Motorola Labs., AZ.

We report on the first direct observation of anisotropic diffusion of large three-dimensional Pt clusters on the anatase TiO_2 (001)-(1×4) surface. Scanning tunneling microscopy (STM) investigation has shown that Pt clusters exhibit narrow size distribution on anatase surface, and that, upon annealing in vacuum, the clusters migrate to step edges via a cluster diffusion mechanism. During this process, the total number of clusters is conserved and the cluster size distribution remains unaltered. These findings imply that no cluster coalescence has taken place for the annealing conditions considered in our study. Inspection of STM images and autocorrelation analysis of the temporal changes in the spatial distribution of clusters on the surface have shown that clusters diffuse on terraces primarily along the atomic rows. The Pt cluster system has been modeled as a non-interacting two-dimensional lattice gas diffusing on a heterogeneous surface with special binding sites (step edges). A one-dimensional model accounting for the statistical variability of terrace dimensions has been used to recover the cluster diffusion coefficient from the temporal changes in terrace cluster population during annealing at several temperatures. The model results show that cluster diffusion on the terraces exhibits Arrhenius temperature dependence. Enforcing the principles of chemical equilibrium between cluster populations on terraces and step edges, coupled with experimental data, yielded the difference in cluster binding energy on terraces and step edges. This binding energy difference is found to be on the order of the activation energy for cluster diffusion and exhibits temperature dependence.

N3.27
PSEUDOHEXAGONAL COMMENSURATE PHASE AT Co/Si(111) INTERFACE.
Tae Soo Kang, Jung Ho Je, POSTECH, Dept of Materials Sci & Eng, Pohang, KOREA; Hyo Jung Kim, Do Young Kim, KJIST, Dept of Materials Sci & Eng, Kwangju, KOREA; Nam Dong Kim, Jin Wook Chung, POSTECH, Dept of Phys, Pohang, KOREA.

The highly strained interfacial structure and reaction of Co on Si(111) in early growth stage was studied by *in-situ* surface x-ray scattering. Cobalt was deposited by e-beam evaporation on reconstruction Si(111) 7 × 7 in ultra high vacuum. Our study reveals that the interfacial layer, formed by the reaction of Co with Si in early growth stage, is a silicide layer with stoichiometry Co_2Si. The silicide layer is a commensurate phase, pseudohexagonal Co_2Si, which has a long-range order imposed by the Si substrate, but large local atomic displacements. Intensity oscillations at the anit-Bragg position during deposition show that a layer-by-layer comsumption of silicon substrate occurs for the first 4 monolayers of cobalt deposited.

N3.28
PROCESS VARIABILITY IN NUCLEATION AND GROWTH OF YSZ CRYSTALS IN COMBUSTION CHEMICAL VAPOR DEPOSITION.
Zhigang Xu, Jag Sankar, Sergey Yarmolenko, Qiuming Wei, NSF Center for Advanced Materials and Smart Structures, North Carolina A&T State University, Greensboro, NC.

Yttria stabilized cubic phase zirconia (YSZ) is an oxygen ion conductive material. It was the electrolyte used in the first solid oxide fuel cell (SOFC). It is still the most effective of the available electrolytes for high-temperature fuel cells. For its best performance, thin film is favored to minimize the current path. In the SOFC, both the air and fuel electrodes are porous materials. The thin film of electrolyte is placed between these electrodes. It has to be gas-tight to avoid any mixing of the oxidant and fuel gases. Only the oxygen ions are allowed to pass through it. Fundamental understandings towards the growth of thin, gas-tight YSZ film on the porous substrates are very important to its successful application. Atmospheric combustion chemical vapor deposition (ACCVD) technique for thin film processing has been developed. Among the advantages are the high growth rate, low setup cost and low run cost. Nucleation and growth of YSZ crystals on different substrates are investigated with the ACCVD technique. The emphases are to understand the effects of lattice misfit, material and surface condition of substrates, and various processing parameters on the nucleation and growth. The methods to enhance the nucleation density and the ability to seal pores on substrate are studied. The evolutions of microstructures from nuclei to continuous films are observed. The microstructures are studied with scanning electronic microscopy and transmission electronic microscopy. The grain size distribution and crystal orientations of both the discontinuous and continuous films are statistically studied.

N3.29
SURFACE RECONSTRUCTION AND INDUCED UNIAXIAL MAGNETIC FIELDS ON Ni FILMS.
R. Alejandra Lukaszew, Brandon McNaughton, Physics and Astronomy Department, University of Toledo, OH; Vladimir Stoica, Roy Clarke, Physics Deparment, University of Michigan, Ann Arbor, MI.

Epitaxial magnetic thin films may be used in a variety of applications such as electrodes in a spin-dependent tunneling junction, so that magnetocrystalline anisotropy can be used to define two states of the magnetization.[1] It is expected that the magnetic properties will be strongly affected by the surface character of the films. In our preliminary work, we prepared epitaxial magnetic films on copper buffer layers grown on silicon substrates.[2]. Films grown at room temperature usually exhibit a rough surface, unsuitable for many technological applications. Thus, usually the films are annealed in order to achieve a smoother surface. One disadvantage in this type of samples is the chemical interaction between the metallic layers and the silicon substrate. In order to explore the possibility of epitaxial magnetic films on less reactive substrates, we have studied the growth on MgO substrates. We have shown that it is possible to obtain epitaxial (001) and (111) Ni films grown on MgO substrates. Uppon annealing, our surface studies on these films indicated the presence of a strain-induced surface reconstruction on the (001) films, while no reconstruction was observed for the (111) oriented ones.[3] Studies on the azimuthal dependence of the magnetization reversal evidenced the presence of a uniaxial anisotropy field superimposed to the expected 4-fould anisotropy due to magnetocrystalline anisotropy in the (001) films while there was not such observation in the (111) films, indicating a strong correlation between the surface reconstruction and the magnetic properties of the films. We will present our subsequent studies on the uniaxial induced anisotropy field using a phenomenological model that successfully accounts for the azimuthal dependence of the magnetization reversal in epitaxial thin films.
[1]R.A. Lukaszew, Y. Sheng, C. Uher and R. Clarke, Appl. Phys. Lett. 75, 1941 (1999). [2]R.A. Lukaszew, Y. Sheng, C. Uher and R. Clarke, Appl. Phys. Lett. 76, 724 (2000). [3]R.A. Lukaszew, V. Stoica, C. Uher and R. Clarke, MRS Proceedings, Fall 2000.

SESSION N4: STRESS RELAXATION
Chairs: Eric A. Stach and Eugene A. Fitzgerald
Tuesday Morning, November 27, 2001
Room 306 (Hynes)

8:30 AM *N4.1
DISLOCATION INTERACTIONS DURING RELAXATION OF ELASTIC MISFIT STRAIN IN THIN FILMS.
L.B. Freund, Division of Engineering, Brown University, Providence, RI.

The critical thickness concept, by which conditions necessary for the formation of the first elastic strain relieving misfit dislocation in an epitaxial film with mismatch are identified, is a cornerstone concept of heteroepitaxy. Here, the interaction of multiple dislocations in a thin film at thickness beyond the critical thickness is discussed, largely on the basis of energy considerations. For the case of a parallel array of dislocations, it is shown that the most common interpretation of the energetics is not consistent with mechanisms of misfit dislocation formation. Next, misfit dislocations on intersecting glide planes is discussed, with focus on the role of the misfit dislocation on one such plane blocking the progress of a threading dislocation on an intersecting plane. Finally, the understanding of the energetics of dislocation arrays is combined with observation on the kinetics of glide of a threading dislocation to arrive at rate equations for overall strain relaxation in a film.

9:00 AM N4.2
STRAIN RELAXATION IN SiGe THIN FILMS STUDIED BY LOW-ENERGY ELECTRON MICROSCOPY.
A.R. Woll, P. Moran, E.M. Rehder, B. Yang, T.F. Keuch and M.G. Lagally, University of Wisconsin, Madison, WI.

The growing technological importance of strain and strain relaxation in semiconductor thin films has highlighted the lack of a comprehensive understanding of strain relaxation mechanisms, such as dislocation creation and motion. Very few tools, other than transmission electron microscopy, are suitable for studying the motion and dynamics of single dislocations. Low-Energy Electron Microscopy (LEEM) is a powerful tool for examining the dynamic evolution of crystalline surface morphology with atomic-height resolution. Changes in surface height caused by vertical glide are readily observed. In

addition, for the case of Si(001), the anisotropic (2×1) surface reconstruction provides a built-in monitor of uniaxial stress, such as that caused by a buried dislocation. We use LEEM to study dislocation motion in $Si_{1-x}Ge_x$/Si thin films, grown on bulk Si(001) and SOI(001) substrates. We have found that the presence of the buried oxide in SOI accelerates plastic relaxation. Our results will be discussed in the context of recent simulations of dislocation dynamics in thin films.

9:15 AM N4.3
RELAXED SiGe FILMS AND HIGH MOBILITY TENSILE Si ELECTRON CHANNELS FORMED ON SILICON ON INSULATOR SUBSTRATES. E.M. Rehder[a], M. Roberts[a], C.K. Inoki[b], T.S. Kuan[b], M.G. Lagally[a], and T.F. Kuech[a], [a]Materials Science Program, University of Wisconsin-Madison, [b]University at Albany, State University of New York.

Relaxed SiGe buffer layers provide the strain control for forming tensile Si-rich and compressive Ge-rich layers. These layers are attractive for forming modulation doped metal oxide field effect transistors (MODFET) operating considerably faster than if produced in conventional Si. The SiGe film relaxation occurs by dislocation formation. The threading dislocations that remain in the film and the final device are the limiting factor. Our work has found that the onset of relaxation, the relaxation rate, the final relaxed state, and the surface crosshatch of a $Si_{0.82}Ge_{0.18}$ film on a silicon on insulator (SOI) substrate is identical to that on bulk Si substrate. The difference is the film threading dislocation density, which has been reduced several orders of magnitude below the $10^7 cm^-2$ found with the bulk Si substrate. During the film relaxation process on bulk Si or on SOI substrates, dislocation-dislocation interactions push numerous dislocations into the substrate. On the SOI substrate these dislocations will reach the amorphous oxide layer where they dissociate. The greatly reduced strain field of the dissociated dislocation prevents dislocation pinning from occurring and ultimately reduces the threading dislocation density. The SOI substrate allows graded buffer layers to reach a higher Ge composition while grading at a faster rate. Film composition and strain is monitored with high resolution X-ray diffraction, while a dislocation revealing etch and transmission electron microscopy are used to observe the dislocation structures. The carrier mobility of these structures is determined from Hall measurements. Thus strained Si layers suitable for electron channels in MODFET structures can be formed directly on an SOI substrate. The faster grading allows the Si layer to be less than a micron from the insulating layer preserving the isolation and reduced parasitic capacitance advantages of the SOI substrate.

9:30 AM N4.4
NUCLEATION AND DYNAMICS OF DISLOCATIONS IN MISMATCHED HETEROSTRUCTURES. Marco Patriarca, Antti Kuronen and Kimmo Kaski, Research Centre for Computational Science and Engineering, Laboratory of Computational Engineering, Helsinki University of Technology, Espoo, FINLAND.

Recent studies of nucleation of dislocations and dislocation dynamics in lattice-mismatched heterostructures have risen a lot of interest due to the technological importance of such structures. Here we have studied the conditions under which dislocation nucleation takes place at the mismatch interface with internal strain for various nano-structure geometries. In particular, we have determined the dependence of the nucleation thresholds on the basic parameters of the crystals (e.g. the amount of mismatch and its sign), the geometry of the nano-structures, and the system temperature. We have also studied the time evolution and the relaxation process of the nucleated dislocations. These studies have been carried out by using the simulation code with a graphical user interface developed at our laboratory. This on-line simulation system allows a real time interactive visualization of the 3-D Molecular Dynamics model of the crystaline systems and, especially, efficiently detects the presence of dislocations and other types of crystal defects, and tracks them by using an algorithm based on potential energy mapping.

9:45 AM N4.5
IDENTIFICATION OF MISFIT DISLOCATIONS PRODUCING RELAXATION OF AlGaN/GaN HETEROSTRUCTURES. David M. Follstaedt, Paula P. Provencio, Jerrold A. Floro, and Sean J. Hearne, Sandia National Laboratories, Albuquerque, NM.

Strained AlGaN alloys grown epitaxially on GaN relax in a very different manner from that of the well-studied cubic heterostructures because the alloy overlayer is in biaxial tension and the crystal structure is hexagonal. Earlier work (Hearne et al, Appl. Phys. Lett. 76, 1534 (2000)) indicates that relaxation initiated during growth by low-density cracking, which was accompanied by formation of misfit dislocations at the interface over the large distances between the cracks. Plan-view TEM examination of misfit dislocations at the AlGaN/GaN interface shows that they have $< 1 - 100 >$ line directions and an in-plane component of Burgers vector along an a axis. High-resolution TEM images of these dislocations viewed end-on in cross section show that they have a component of their Burgers vector along the c axis. These observations are consistent with misfit dislocations having b = a c and lying on {11-22} glide planes. Moreover, we have independently found such dislocation glide on {11-22} planes in other GaN material, confirming that this is an active slip system. These results now allow us to explain the presence of the misfit dislocations by the nucleation of half-loops at the AlGaN surface where fracture occurred and subsequent glide of threading segments on {11-22} planes to lay misfit segments at the interface.

10:30 AM *N4.6
CHALLENGES IN PERFECTING LATTICE-MISMATCHED EPITAXIAL GROWTH. E.A. Fitzgerald, MIT, Dept of Materials Science and Engineering, Cambridge, MA.

Heteroepitaxial growth of lattice-mismatched semiconductors has enabled new commercial device technologies, such as III-V bipolar transistors, HEMTs, and SiGe bipolar transistors. These devices can have advantages due to strained, unrelaxed semiconductor layers, and they are a direct result of early work in the 1980's that explored concepts such as the critical thickness for misfit dislocation introduction. We are now moving into a period in which relaxed lattice-mismatched layers can have a potentially larger impact commercially, but new issues in lattice-mismatched heteroepitaxial growth arise. In this talk, we will review our research regarding dislocation relaxation in lattice-mismatch semiconductors in the SiGe/Si, InGaAs/GaAs, and InGaP/GaP systems. Common traits and differences in these systems will be presented. Time permitting, we will describe how commercialization of lattice-mismatched materials can impact Si CMOS technology as well as III-V electronics and optoelectronics.

11:00 AM *N4.7
LOW ENERGY PLASMA ENHANCED CHEMICAL VAPOUR DEPOSITION. Carsten Rosenblad, Matthias Kummer, Elisabeth Müeller, Hans von Känel, Laboratorium für Festkörperphysik, ETH-Zürich, Zürich, SWITZERLAND; Thomas Hackbarth, DaimlerChrysler Research & Technology, Ulm, GERMANY; Georg Höck, Department of Electron Devices and Circuits, University of Ulm, Ulm, GERMANY; Alex Dommann, Interstate University of Applied Science NTB, Buchs, SWITZERLAND.

Using a low voltage but high current DC plasma discharge, we have recently implemented a new growth process for the deposition of epitaxial Si and SiGe. With ion energies below 15 eV, epitaxial material is deposited without any accompanying ion damage, from which the name "Low energy plasma enhanced chemical vapour deposition" (LEPECVD) is derived. The high discharge current allow for exceptionally high growth rates of at least 10 nm/s, independent of the substrate temperature in the range 500°C - 750°C. The high growth rates makes LEPECVD particularly suited for the synthesis of thick epitaxial layers. The compositionally graded SiGe relaxed buffer layer is an example to which we have paid particular interest. The high quality of such relaxed buffer layers will be demonstrated, and examples of complete high mobility SiGe hetero-FETs will be discussed.

11:30 AM N4.8
DYNAMICS OF DISLOCATIONS AND SURFACE INSTABILITIES IN MISFITTING HETEROEPITAXIAL FILMS. Mikko Haataja, Department of Mechanical and Aerospace Engineering and Princeton Materials Institute, Princeton University, Princeton, NJ; Judith Muller, Instituut-Lorentz for Theoretical Physics, University of Leiden, Leiden, THE NETHERLANDS; A.D. Rutenberg, Department of Physics, Dalhousie University, Halifax, CANADA; Martin Grant, Centre for the Physics of Materials, Department of Physics, McGill University, Montreal, CANADA.

We introduce a continuum model of elasticity in a nonequilibrium multiphase system - including smooth and singular strains, as well as their coupling to free surfaces - and apply it to the dynamics of misfitting heteroepitaxial films. Above a critical thickness dislocations relieve strain, competing with an instability at the interface. At early times, the initial untable growth of interface fluctuations is driven by an effective misfit strain which in turn depends on the dislocation mobility and density. At late times, our results show that the interaction between singular and smooth strains leads to complicated morphologies. Depending on their mobility, dislocations can screen stress by building up at large-curvature groove tips, leading to high ductility, or they can be "outrun" by the tips, leading to brittleness.

11:45 AM N4.9
X-RAY ANALYSIS OF Si/Ge/Si(001) HETEROLAYER STRUCTURES GROWN BY SURFACTANT MEDIATED EPITAXY. B.P. Tinkham, W.P. Rodrigues, D.M. Goodner, D.A.

Walko and M.J. Bedzyk, Department of Materials Science and Engineering, Northwestern University, Evanson, IL.

We have used X-ray Standing Waves, X-ray Reflectivity, and Grazing Incidence X-ray Diffraction for a structural analysis of ultra-thin Si/Ge/Si(001) heterostructures grown by surfactant mediated molecular beam epitaxy. Both Bi and Te were used as surfactants and we compared samples of varying Ge thickness to determine the extent to which one can grow strained layers of Ge on Si(001). Specular X-ray reflectivity was performed at low angle and in the vicinity of the Si(004) bragg peak to determine interfacial roughness between layers. The Grazing Incidence X-ray Diffraction measurements enabled us to control the scattering depth of the x-rays, thus allowing us to measure the degree of strain (or relaxation) in the Ge epilayer. X-ray Standing waves (XSW) is a complementary technique that we use to measure the registry of the Ge atoms with respect to the Si substrate lattice. For samples grown without surfactant the XSW coherent fraction and position of Ge are markedly lower than for samples of similar thickness grown with both Te and Bi as a surfactant. Using continium elasticity theory we provide different structural models to interpret this behavior. In addition, by performing XSW measurements at both Si(004) and Si(008) Bragg peaks we were able to determine the disordered fraction in the buried Ge thin films.

SESSION N5: STRESS AND ISLANDING
Chairs: Allan F. Bower and Jerrold A. Floro
Tuesday Afternoon, November 27, 2001
Room 306 (Hynes)

1:30 PM *N5.1
MORPHOLOGICAL EVOLUTION DURING SiGe/Si STRAIN LAYER EPITAXY. Jerrold A. Floro, Sandia National Laboratories, Albuquerque, NM; Jennfier L. Gray and Robert Hull, University of Virginia, Dept. of Materials Science and Engineering; Eric Chason, Div. of Engineering, Brown University, Providence, RI.

Strain relaxation in heteroepitaxial layers often occurs via a competition between misfit dislocation introduction and 3D surface morphological evolution. These processes are being exploited for self-assembly of quantum dot structures with applications in optoelectronics, magnetics, and perhaps in novel logic applications. This talk will first overview morphological evolution processes occurring in SiGe alloys grown by MBE on Si under conditions of very high adatom mobility. In these experiments, the film stress, as well as the island size, spacing, and lateral ordering are measured in situ, in real-time via novel optical diagnostics. From this data we can obtain the kinetics of island coarsening directly, where it is found that the coarsening rate accelerates as the islands become larger. This unusual ripening process can be explained through the effect of inter-island elastic repulsion, combined with a growth flux, on Ostwald ripening processes. The second portion of the talk will cover recent measurements of SiGe/Si morphological evolution under conditions of intermediate adatom mobility. Within a relatively narrow range of growth conditions, preferential nucleation of pits occurs to relieve strain, followed by cooperative nucleation of contiguous island "rings" surrounding the pits. Misfit dislocations eventually enter the film, whereupon the < 100 >-oriented coherent ring structures disappear and are replaced by < 110 >-oriented cross-hatch. 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.

2:00 PM N5.2
STRAIN RELAXATION IN Ge DOMES GROWN ON Si (001). R. Magalhães Paniago, Depto. de Física, ICEx, Universidade Federal de Minas Gerais, Belo Horizonte, MG, BRAZIL; G. Medeiros-Ribeiro, Laboratório Nacional de Luz Síncrotron, Campinas, SP, BRAZIL, and Hewlett-Packard Labs, Palo Alto, CA; S. Kycia, Laboratório Nacional de Luz Síncrotron, Campinas, SP, BRAZIL; T.I. Kamins and R. Stanley Williams, Hewlett-Packard Labs, Palo Alto, CA.

Epitaxial growth of Ge on Si (001) produces a wealth of morphologies, and it has been the subject of intense investigation in the past years. Of the many morphologies that can be produced, coherent island formation is one that is heavily studied, as it represents a simple system to model self-assembled nanocrystal growth. The shape transition observed in this system [1], specifically the pyramid to dome transition, has been modeled and the strain relaxation on these structures evaluated by plan-view transmission electron microscopy [2]. In this work, x-ray scattering experiments on monodisperse, single shape islands ensembles are presented. Most specifically, the mean lattice parameter is measured as a function of the island diameter at the XD1 beam line at the LNLS, the Brazilian Synchrotron light source. The size dispersion was evaluated by Atomic Force Microscopy (AFM) where careful statistical analysis was performed on the same samples as used in the x-ray scattering experiments. Through the AFM statistics, a relationship between the island diameter and height was obtained, and from that and the x-ray data we could infer the strain relaxation as a function of the vertical position in the island. From these experiments we obtained the relaxation profiles as a function of the in-plane direction, and were able to map that onto the bounding facets of these multifaceted nanocrystals. [1] G. Medeiros-Ribeiro, A.M. Bratkovski, T.I. Kamins, D.A.A. Ohlberg, and R.S. Williams, Science 279, 353 (1998); F.M. Ross, J. Tersoff, R.M. Tromp, Phys. Rev. Lett. 80, 984 (1998) [2] Chuan-Pu Liu, J. Murray Gibson, David G. Cahill, Theodore I. Kamins, David P. Basile, and R. Stanley Williams, Phys. Rev. Lett. 84, 1958 (2000).

2:15 PM N5.3
STRESS IN Ge DOTS ON Si(001) BY REALISTIC SIMULATIONS. Paolo Raiteri and Leo Miglio, INFM and University of Milano-Bicocca, Dept. of Materials Science, Milano, ITALY.

We report very recent, still unpublished results on a quantitative estimate of the strain, stress and elastic energy at realistic Ge dots on Si (001) by molecular dynamic simulations with a Tersof potential. In particular, we show how much strain relaxation in the dot depends on the dot morphology (105 pyramid, 103 pyramid and dome) and size (from 5 to 38 nm). The role of the elastic energy in the Ge wetting layer (2x8 reconstructed) and in the Si substrate (more than 8 nm in our model) is also demontrated to be an important issue in understanding the limitation in dot size and self-assembling.

2:30 PM N5.4
SHAPE TRANSITIONS OF SELF-ASSEMBLED Ge ISLANDS ON Si(001). Armando Rastelli, INFM - Dip. di Fisica A. Volta, Univ. di Pavia, Pavia, ITALY; Hans von Känel, Matthias Kummer, Lab. für Festkörperphysik, ETHZ, Zürich, SWITZERLAND.

Three-dimensional Ge islands were grown on Si(001) by ultra high vacuum (UHV) magnetron sputter epitaxy. Atomic scale investigations as well as a statistical analysis of the island size and shape evolution were performed by UHV scanning tunneling microscopy (STM). During Ge deposition at a substrate temperature $T_s = 550°C$, coherently strained islands undergo several shape transitions [1] as their volume exceeds certain critical values. They change from small stepped mounds (*prepyramids*) to {105} faceted *pyramids* and eventually to multifaceted *domes*. The transitions are gradual and involve islands with intermediate shape like truncated pyramids or pyramids with stepped facets. A complete reversal of this pathway has been observed during the overgrowth of the Ge islands with thin ($0.1 - 3$ nm) layers of Si at $T_s = 450°C$. Islands with different shape and size are found to transform to their precursors at different stages of the Si capping: small pyramids and domes display appreciable changes at coverages lower than one monolayer (0.14 nm), while larger islands of each shape start their back-transformation at higher coverages. The Si cap, necessary for the potential exploitation of the islands as quantum dots, efficiently intermixes with Ge leading to a strain reduction and driving the transitions. Those observations suggest that the shape of an island is mainly determined by its volume and misfit with the substrate and can be understood in a coherent picture unifying the behaviour of the Ge/Si system with the less mismatched Ge_xSi_{1-x}/Si. The presented results are expected to be of relevance also for other self-assembled systems displaying shape transitions. [1] A. Vailionis et al., Phys. Rev. Lett. 85, 3672 (2000). F.M. Ross et al., Science 286, 1931 (1999). J.A. Floro et al., Phys. Rev. B 59, 1990 (1999). G. Medeiros-Ribeiro et al., Science 279, 353 (1998).

2:45 PM N5.5
EVOLUTION OF STRESS AND RELAXATION OF STRAIN OF Ge AND GeSi ALLOY FILMS ON Si(001). Reinhold Koch, Paul-Drude-Institut für Festkörperelektronik, Berlin, GERMANY; Bernhard Wassermann, Gerd Wedler, Freie Universität Berlin, GERMANY.

The growth of Ge and GeSi alloy films on Si(001) has attracted considerable interest in the last years because of their importance for optoelectronic devices as well as Si-based high speed transistors. Here we report on real time stress measurements by a sensitive cantilever beam technique in combination with in situ structural investigations by scanning tunneling microscopy at deposition temperatures of 800 - 1000 K. Characteristic features in the stress curves provide detailed insight into the development and relief of the misfit strain as well as the respective growth mode. For the Stranski-Krastanow-system Ge/Si(001) the strain relaxation proceeds mainly in two steps: (i) by the formation of 3D islands on top of the Ge wetting layer and (ii) via misfit dislocations in larger 3D islands and upon their percolation. Co-deposition of Si influences the stress behavior drastically. The growth mode changes from Stranski-Krastanow to a kinetic 3D island mode at Si concentrations of about twenty percent leading to the so far smallest quantum dots of the Ge/Si system.

3:30 PM *N5.6
NUMERICAL SIMULATIONS OF ISLAND NUCLEATION AND GROWTH IN STRAINED HETEROEPITAXIAL THIN FILMS.
A.F. Bower, Division of Engineering, Brown University, Providence, RI; Y.W. Zhang, NUS, SINGAPORE.

The spontaneous nucleation and growth of islands during deposition of a strained heteroepitaxial thin film offers an appealing technique to manufacturing quantum dots. In this paper, we describe detailed numerical simulations of self-organization in arrays of strained islands. Our analysis accounts for the effects of elastic and surface energy anisotropy, strain relaxation, the wetting layer, and interactions between neighbouring islands, as well as the kinetics of mass transport and deposition on the surface. The model is used to conduct detailed parametric studies of the influence of elastic and surface properties, growth temperature and deposition rate on the size, shape and spatial distribution of islands. Conditions that optimize the uniformity of spatial and size distributions of islands are identified. In addition, the role of surface energy anisotropy and elastic interactions on shape transitions in islands is studied in detail. We find that small islands tend to adopt a hut shape, while larger islands are domed, in agreement with experiment and existing models. The volume of a stable hut can be larger than that of a stable dome, however, indicating that there is an energy barrier to the hut-to-dome transition. The critical conditions for shape transition during growth are determined by the stability of a hut-shaped island, therefore, not only by energy changes associated with the transition. We find that an isolated hut-shaped island becomes unstable if it exceeds a critical volume, which depends strongly on the nature of the anisotropy in surface energy. Interactions between neighbouring islands reduce the critical volume: in particular, impingement between islands nucleates new facets at the island base, which subsequently triggers a shape transition.

4:00 PM N5.7
SHAPE TRANSITION IN SELF-ORGANIZED InAs/InP NANOSTRUCTURES.
H.R.Gutiérrez, M.A. Cotta and M.M. G.de Carvalho, UNICAMP, Instituto de Física Gleb Wataghin, DFA/LPD, Campinas-SP, BRAZIL.

InAs/InP nanostructures have received much attention in recent years. Different InAs shapes (wires and dots) grown on InP substrates have been reported so far. Recent results suggest that the surface morphology or the chemical composition of the buffer layer are determinant in configuring the final shape of the InAs nanostructures. However, the mechanisms that originate each kind of structure are not clear. In this work we report the conditions that determine the InAs shape transition - from wires to dots - for films grown on (001) InP surfaces by Chemical Beam Epitaxy. InAs growth evolution was monitored by Reflection High Energy Electron Diffraction (RHEED). The samples were analyzed by Atomic Force Microscopy (AFM) using C-nanotube tips and High Resolution Transmission Electron Microscopy (HRTEM). We observe that the shape transition is obtained when the wires are annealed at growth temperature. The transition was obtained for both nominal and vicinal (2° off) substrates. Moreover, the transition was observed independently of the InP buffer layer morphology (smooth or rippled). RHEED measurements show that the angle of the chevron streaks along the $[1\bar{1}0]$ direction remains stable after 2.5 monolayers. This result correlates well to the facets measured by HRTEM in the InAs wires. On the other hand wires are not observed when InAs is formed by As-P exchange only. Our results suggest that the wires are a metastable shape originated by the anisotropic diffusion over the InP buffer layer during the formation of the first InAs monolayer, which evolves to a more stable shape (dots) during annealing. The driving force for the shape transition is related to the height inhomogeneities along the wire that produce variations in the elastic energy and hence in the chemical potential. The chemical potential gradients may induce a diffusion current to the higher regions originating the dots formation. *Work partially performed at LME/LNLS (Brazil).

4:15 PM N5.8
A CONTINUUM MODEL FOR THE GROWTH AND RELAXATION OF EPITAXIAL THIN FILMS.
Simon Gill, Fei Long, Alan Cocks, Dept of Engineering, University of Leicester, Leicester, UNITED KINGDOM.

The large elastic strains in epitaxial thin films can be relaxed via morphological change of the surface of the film, compositional variation within the film/substrate, and the nucleation of dislocations. The former two relaxation processes are vital to the development of nanoscale self-organised structures, such as quantum dots, and are the subject of this paper. Quantum dots are of practical interest due to their unique electronic properties. These properties are functions of their shape, composition and distribution. It is these quantities that are investigated here using a variational continuum model. A particular feature of quantum dots is their strongly facetted shape. The effect of surface energy anisotropy on shape is analysed and it is found that a number of classes of anisotropy functions can produce similar final states. However, further study shows that the evolution path to these states is strongly influenced by the choice of anisotropy function, and hence the function class has to be chosen carefully. Comparison with experimental observations of InAs dots grown on GaAs supports the choice of an anisotropy function with cusped energy minima. Simulating the evolution of more realistic alloyed quantum dots introduces significantly greater complexity to the model. A two-component model for surface diffusion is presented with some initial results on the compositional evolution of elastically strained thin film surfaces and the formation of alloyed InGaAs dots.

4:30 PM N5.9
STM CHARACTERIZATION OF Ge NANOSTRUCTURES GROWN ON Si(111).
Federico Rosei, Institute of Physics and Astronomy and CAMP, Aarhus, DENMARK; Anna Sgarlata and Nunzio Motta, Dipartimento di Fisica, Univ. Tor Vergata, Roma, ITALY.

We have studied by Scanning Tunneling Microscopy (STM) the formation and evolution of 3 D islands obtained by Physical Vapor Deposition of Ge on Si(111) in the temperature range 450 - 550°C. The early stages of growth has been followed by an STM "movie" showing the formation of triangular, flat islands that progressively increase in density and dimension, up to the completion of the Wetting Layer (WL). This was done by scanning the surface while evaporating Ge at low flux on the Si(111) surface. On this WL 3D coherent island nucleation begins at a Ge coverage between 3 - 5 MonoLayers (ML), depending on the conditions. At T = 500°C the islands (average lateral dimensions 150 - 200 nm) nucleate appear as truncated tetrahedra. The islands evolve firstly by introducing new crystallographic faces and by becoming more rounded in shape, and subsequently by including dislocations at their border, partially relieving the misfit strain. Finally an erosion of the islands' top and of the substrate around the islands occurs, probably connected to a substantial Ge-Si intermixing. This is consistent with previous X-Ray Absorption Fine Structure (XAFS) measurements. We have analyzed the self-organization of the islands, observing that two different growth regimes arise: initially the islands form and evolve only on the steps, up to complete ripening; subsequently the same happens on flat areas of the sample. For Ge deposited at 450°C, the average distance between islands and steps is nearly constant, forming initially a single row of equally spaced islands, followed by rows in between. A controlled exploitation of this phenomenon, governed by the surface diffusion coefficient of Ge on Si (which we estimate from data analysis), is one possible path to achieve controlled self-organization of quantum dots, leading to nanoscale integration on a single Si "chip".

4:45 PM N5.10
MORPHOLOGIES OF SELF-ASSEMBLED QUANTUM DOTS: A VARIATIONAL APPROACH.
R. Arief Budiman and Harry E. Ruda, Centre for Advanced Nanotechnology, University of Toronto, Toronto, Ontario, CANADA.

We construct a model for coherent island formation by (i) using a novel 3D strain tensor that accounts for the bulk, varying elastic strains of a thin film, and (ii) representing adatom diffusion as an external field that perturbs an otherwise flat film. Equilibrium shapes of islands are obtained by minimizing the total free energy with respect to the shear strains along growth direction. These strains were also determined to be the order parameter for the islanding transition. Transition thicknessthe wetting layer thickness at the onset of the islanding transitionis obtained by minimizing the free energy with respect to the longitudinal strain along the growth direction. Comparison with MBE- and CVD-grown $Si_{1-x}Ge_x$/Si(001) islands will be discussed in detail.

SESSION N6: MODIFYING AND CONTROLLING GROWTH
Chairs: Eric H. Chason and Max G. Lagally
Wednesday Morning, November 28, 2001
Room 306 (Hynes)

8:30 AM *N6.1
SELF-ASSEMBLY AND STRAIN ENGINEERING OF Ge/Si(001) HETEROEPITAXIAL FILMS AND QUANTUM DOTS.
Max G. Lagally, University of Wisconsin-Madison, Madison, WI.

Future generations of micro- and optoelectronic devices may require approaches beyond the conventional in terms of materials fabrication and integration at the nanoscale. In materials integration - combining different materials to increase the function of each - two approaches dominate: materials bonding and heteroepitaxy. In heteroepitaxy the resulting strain fields can cause the formation of small, dislocation-

free, perfect, 3D islands spontaneously during growth to relieve lattice mismatch stress through elastic deformation. Frequently, however, we don't want 3D structures, but flat films. In particular in the SiGe system, high-Ge-concentration SiGe films are desirable for some device applications. Strain management in the growth of SiGe films therefore has two potentially opposing goals: make flat films or make perfectly arranged, uniformly sized QDs. Because SiGe is only a two-component system, achievement of these opposing goals requires novel approaches to strain management. We describe recent efforts we have made in controlling film growth (via both MBE and CVD), QD self assembly, and dislocation formation in SiGe. These include use of lateral pattering, silicon-on-insulator (SOI) substrates, and application of external stress using MEMS devices. We use RHEED, LEEM, AFM, STM, and XRD to analyze structure, morphology, and growth evolution of the films. We present recent electrical measurements in device structures containing layers of SiGe dots to demonstrate the potential of SiGe QD devices. Research supported by NSF and DARPA. Work done in collaboration with D. Savage, P. Rugheimer, E. Rehder, T. Kuech, F. Flack, A. Woll, and M. Eriksson.

9:00 AM N6.2
DIRECTED MORPHOLOGICAL EVOLUTION OF THIN FILMS DURING HETEROEPITAXY. J.J. Eggleston and P.W. Voorhees, Dept. of MS&E, Northwestern University, Evanston, IL.

We examine the evolution of a misfitting film during heteroepitaxy in an effort to develop methods that can be used to control the size distribution and arrangement of islands on surfaces. The film is assumed to evolve by deposition, and surface diffusion in response to the interfacial and elastic energies of the system. The phase field model allows for both isotropic surface energy and highly anisotropic surface energy where the equilibrium shape has corners and edges. We find that highly anisotropic surface energy dramatically increases the rate of island formation. We examine the effects of mesas on the evolution of the film. We show that islands can form at the edges of a mesa due strictly to capillarity driven surface diffusion. However, when a misfit is present and the surface energy is isotropic, the mesa induces a travelling wave that propagates parallel to the substrate and perpendicular to the mesa with a wave speed that is much faster than the growth rate of the ATG-instability. This, in turn leads to a narrower size distribution of the resulting islands than in systems without a mesa and a means of tailoring the spatial arrangement of islands on a surface.

9:15 AM N6.3
NON-LITHOGRAPHIC FABRICATION OF SnGe QUANTUM WIRES BY MOLECULAR BEAM EPITAXY. Regina Ragan and Harry A. Atwater.

SnGe alloys are a class of group IV materials that exhibit a direct energy bandgap. We have previously reported an indirect to direct energy gap transition for compositionally homogeneous SnGe alloys with $x > 0.11$.[1] However, the incorporation of Sn in a Ge matrix is not thermodynamically favorable due limited bulk solid solubility as well as a strong tendency for Sn atoms to segregate to the surface during MBE growth. The resulting phase separation observed in molecular beam epitaxy of approximately 1 micron thick SnGe alloy thin films, while unfavorable for homogeneous alloy formation, can be utilized in the formation of dense arrays of SnGe quantum wires oriented perpendicular to the substrate plane. During epitaxial growth of SnGe alloys on Ge(001) at T = 160°C and growth rate of 3 nm/min, a modulation of the alloy composition develops perpendicular to the film-substrate interface evident in transmission electron microscopy for film thickness equal to 1 um. For the SnGe alloy with x = 0.03, the lateral composition modulation has a period of 40-50 nm. The experimentally measured period of the composition modulation is compared with existing thermodynamic theory[2] which is a function of both composition and strain. Further analysis of Scanning transmission microscopy in planar view yields a Sn composition in the Sn-rich wires of approximately x =0.05. Transmission electron microscopy analysis indicates that the phase separation is occurring within coherent films and is not related to dislocation formation. FTIR spectroscopy of these phase separated alloys has an absorption edge dominated by the Sn rich regions. Optical and structural characterization of 1 micron phase separated SnGe alloys will be presented. [1]G. He and H.A. Atwater, Phys. Rev. Lett. 79, 1937 (1997) [2]F. Glas, Phys. Rev. B 55, 11277 (1997).

9:30 AM N6.4
INTERFACE ENGINEERING IN TYPE II CdSe/BeTe QUANTUM DOTS. Sergey Ivanov, Tania Shubina, Alexey Toropov, Sergey Sorokin, Reginald Kyutt, Alla Sitnikova, Ioffe Physico-Technical Institute of RAS, St. Petersburg, RUSSIA; Magnus Willander, Chalmers University of Technology and Goteborg University, Goteborg, SWEDEN; Andreas Waag, Abteilung Halbleiterphysik, University of Ulm, Ulm, GERMANY; and Gottfrid Landwehr, Physical Institute of Wuerzburg University, Wuerzburg, GERMANY.

It has been shown recently that self-organization of CdSe/ZnSe based nanostructures grown by MBE is characterized by significant vertical broadening of CdSe-enriched islands (up to 10 monolayers (ML)). Along with relatively large lateral sizes of the islands it makes difficult to consider the quantum disk-like Cd compositional fluctuations in the disordered ZnCdSe alloy as quantum dots (QDs). Therefore, looking for new approaches differing from the Stranski-Krastanow growth mode to controllable fabrication of real II-VI QDs having well defined interfaces and being optically active up to room temperature is of great importance. The main idea of the novel technique developed and presented in this paper is an intentional introduction of a super-strained fractional monolayer (FM) of a much stronger lattice-mismatched compound – stressor – to create strong local stress fields on the matrix surface immediately before deposition of the QD material. The study is performed on MBE grown type II CdSe/BeTe nanostructures of no-common-atom binaries ($\Delta a/a \sim 7\%$), exhibiting weak interdiffusion of constituent atoms and allowing careful optical examination of the interface chemical bonds due to strong in-plane photoluminescence (PL) anisotropy induced by possible non-equivalence of the interfaces [2]. Intentional growing of 0.1-0.2 ML thick CdTe FMs at both CdSe/BeTe interfaces, carefully monitored by RHEED, has allowed us to control both intrinsic morphology evolution of CdSe islands from disk-like to 0D QDs (<5 nm) and dominant interface bond at the same CdSe nominal thickness. Both BeSe ($\Delta a/a \sim -10\%$) or CdTe ($\Delta a/a \sim 14\%$) interface monolayers may be formed in the basement of the island depending on amount of the CdTe deposited. Structural properties and the interface composition of the multilayer structures with a CdSe nominal thickness varied in the 0.4-1.5 ML range and ~5 nm BeTe barriers were studied using transmission electron microscopy and detailed simulation of x-ray diffraction curves. The possibility to obtain bright room-temperature PL is demonstrated. The developed approach may be extended to other II-VI QD systems. [1] N. Peranio et al., Phys. Rev. B 61 (23), 16015 (2000). [2] T.V. Shubina et al., Proc. ICPS 25, Ocaka, 2000, p. 1293.

9:45 AM N6.5
SURFACTANT-INDUCED GROWTH OF Ag ON Cu(111): A LOW ENERGY ION BEAM SCATTERING STUDY. K. Umezawa, T. Tatsuta, S. Nakanishi, Dept. of Materials Sciences, Osaka Prefecture University, Sakai, Osaka, JAPAN; W.M. Gibson, Dept. of Physics, University at Albany, SUNY, Albany, NY.

Using 2 keV-$^{20}Ne^{+}$ ions, low energy ion beam scattering analysis has been applied to a study of Ag on Sb-precovered Cu(111). The Ag and Sb evaporation rates are verified by RBS measurements using 2 MeV-4He. It has been shown that submonolayer deposits of Sb change the growth mode of Ag(111). A layer-by-layer growth behavior was observed at the deposition temperature at RT. However, the growth mode of Ag(111) is different from that on Cu(111) without Sb adatoms. In previous works, we showed that two different types of epitaxial growth exist: Ag[11-2]//Cu[11-2] (type-n) and Ag[-1-12]//Cu[11-2] (type-r) [1-3]. The growth modes of the Ag thin films on Cu(111) surfaces depend strongly on the temperature during deposition with the Ag(111) planes having a preferred orientation of either type-n or type-r growth mode as a function of the Cu substrate temperature. Simulation results for the spectrum show that type-n vs. type-r mode abundance are 23% and 77%, respectively at RT. On the other hand, with 0.2 ML of Sb, type-n vs. type-r mode abundance of Ag(111) planes dramatically change 50% and 50%, respectively at RT. Moreover, the embedded Sb atoms segregate to the newly formed layer, and occupy hcp hollow sites to the underlying Ag(111) planes. The surfactant effects of Sb atoms would reduce the Ag adatoms mobility, and give rise to a smooth growth. [1] K. Umezawa, S. Nakanishi, M. Yoshimura, K. Ojima, K. Ueda, W.M. Gibson, Phys. Rev. B 63 (2001) 035402. [2] K. Umezawa, S. Nakanishi, and W.M. Gibson, Surf. Sci. 426 (1999) 225. [3] K. Umezawa, S. Nakanishi, and W.M. Gibson, Phys. Rev. B 57 (1998) 8842.

10:30 AM *N6.6
SUPERSONIC MOLECULAR BEAM EPITAXY AND ATOMIC-LEVEL TEMPLATING OF MATERIALS GROWTH. Steven J. Sibener, The James Franck Institute and Dept. of Chemistry, The University of Chicago, Chicago, IL.

This presentation will focus on two topics: (i) the emerging application of supersonic molecular beams for the epitaxial growth of advanced materials and (ii) the guided assembly of highly-organized nanostructures *via* interfacial templating. The first topic will examine how high kinetic energy supersonic beams can influence thin film growth chemistry of c-SiC, especially with respect to improved morphology, the use of lower growth temperatures, and the delineation of efficient growth mechanisms. The second topic will highlight recent work from our group on the formation and characterization of ordered structures having either atomic or nanoscale periodicities on vicinal surfaces. Time-lapse elevated-temperature STM experiments play a

vital role in these investigations. Illustrative examples will include unusual Xe structures grown on intentionally designed substrates and linear nanostructures consisting of atomic chains of Si epitaxially grown on vicinal metals. Kinetic processes will be shown to significantly influence the degree of perfection achieved in forming vicinal templates and associated overlayers.
*It is with great pleasure that I acknowledge my collaborators: Seth Darling, Aubrey Hanbicki, Tom Pearl, Aaron Rosenbaum, Errol Sanchez, and Yi Wang.
This work was supported by the AFOSR, DOE, and NSF-MRSEC at The University of Chicago.

11:00 AM N6.7
MORPHOLOGY OF SELF-ASSEMBLED InAs QUANTUM DOTS ON GaAs(001). F. Arciprete, F. Patella, S. Nufris, M. Fanfoni, E. Placidi, A. Balzarotti, Dept. of Physics, University of Rome "Tor Vergata" - INFM, Rome, ITALY.

Self-assembled InAs quantum dots grown on GaAs(001) by molecular beam epitaxy (MBE) have been investigated by Atomic Force Microscopy (AFM) and Scanning Tunneling Microscopy (STM). Two different growth procedures have been applied, namely, the usual continuous growth (CG) and the migration-enhanced growth (MEG). In the latter the migration length L_d of indium is enhanced by cycling the total evaporation by means of growth interruptions. Two sets of samples have been grown for InAs coverages, above the critical thickness ($\approx$ 1.7 ML), ranging from 1.7 to 3.0 ML. The results evidence marked differences in the evolution of nanoparticles density and volume; despite of the same set of growth parameters were used. Moreover a marked difference does exist in the wetting layer and/or substrate participation to the two- to three-dimensional transition, as inferred by the dot total-volume analysis. The different morphologies obtained substantiate the important role of kinetics on the thermodynamics in the nonequilibrium MBE growth. At the same time some general features predicted by the equilibrium phase diagram of the mismatched heteroepitaxial growth are indeed observed. The wetting layer and the precursor 2D-islands, for coverage smaller (1.3 ML) than the critical thickness, have been imaged by STM with atomic resolution. A possible intermixing between substrate and wetting layer is discussed in comparison with the STM topographies of a strained $In_{0.2}Ga_{0.8}As$ alloy grown in the same conditions. The evolution of surface morphology during the 2D to 3D transition has also been studied in the range of 1.3-1.9 ML of InAs coverages. It is characterized by the coexistence of 2D islands and a bimodal size distribution of 3D islands, which evolve toward a monomodal one for coverages higher than 1.9 ML.

11:15 AM N6.8
OXIDATION BEHAVIOUR OF SELF-ASSEMBLED DOTS OF Ge ON Si(001). Torsten Sass, Vilma Zela, Ines Pietzonka and Werner Seifert, Solid State Physics, University of Lund, SWEDEN.

Oxidation and subsequent selective reduction of self-assembled islands of Ge grown on Si might provide one way to create Ge-dots embedded into an insulating material. We have studied the formation of a dot-population of only dome-shaped islands with high size homogeneity (typically 70 nm in width and 15 nm in height) by step-wise deposition of germanium. The formed surfaces were exposed to (a) oxygen plasma at room temperature and (b) saturated water-vapour at different temperatures. The results of the oxidation process were studied by high-resolution transmission electron microscopy. In case (a) the oxygen plasma turns out to remove unselectively material from the whole surface. Thereby the effective height of the oxidized Ge islands increases in relation to the Si oxide layer covering the area between the Ge islands. In case (b) saturated water-vapour in nitrogen carrier gas was applied for 30 minutes at temperatures of 500, 600, 650 and 700°C. It was found that, with the exception of the lowest temperature, the Ge islands are completely converted into oxide. The most remarkable effect is the variation of the thickness of the produced Si-oxide in the vicinity of the Ge dots. It is thinnest close to the corners of the Ge islands, whereas it is thickest directly underneath the Ge islands. Thus, the Si oxide thickness reflects the strain situation, with compressive strain at the corners and tensile strain underneath the Ge islands. The oxidation of Si underneath the Ge islands is due to diffusion of water through the oxidized islands. Only the oxidation at 500°C produces no oxide underneath the islands and a Si oxide of about 2.5 nm thickness outside the islands. The oxide-thickness versus temperature plot shows increased oxidation rates for the Si-surface in these structures in comparison to bulk Si.

11:30 AM N6.9
ISLAND AND PIT FORMATION DURING GROWTH AND ANNEALING OF InGaAs FILMS. A. Riposan, M. Bouville, M.L. Falk and J. Mirecki Millunchick, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI.

We studied the morphological evolution of intermediately strained alloys in the III-V system, focusing on the initial stages of 3D roughening. A series of $In_{0.27}Ga_{0.73}As$ films (lattice mismatch f = 1.9%) were grown on GaAs (001) using Molecular Beam Epitaxy under various growth conditions. The surface morphology near the onset of 3D roughening was investigated for films immediately after growth and after annealing. There are several morphological regimes: layer-by-layer, roughening, and 3D growth. As expected, 3D island nucleation coincides with the onset of strain relaxation at a critical thickness h_c, as measured by Reflection High Energy Electron Diffraction. As strain relaxation continues, pits form adjacent to clusters of 3D islands. The onset of the pit formation depends on the growth conditions, including growth temperature and As overpressure, and the density of 3D islands. In the $In_{0.27}Ga_{0.73}As/GaAs$ system, both the islands and the pits are aligned along the $[1\bar{1}0]$ direction, and appear to be bound by {136} faces. The islands and pits coalesce into ripple arrays as the film thickness increases. Films slightly below and above the critical thickness for 3D roughening were annealed to study the stability of islands and pits. For films with thicknesses below h_c, initially smooth surfaces evolve into islanded morphologies upon annealing. Films grown slightly above h_c have both islands and pits on the surface. Upon annealing, the pits disappear and the islands coalesce into ripples. We will discuss these results in terms of a kinetic model that takes into account the interactions of adatoms, surface steps, islands and pits.

11:45 AM N6.10
SELF-ASSEMBLED InAs QUANTUM WIRES ON InP(001). Haeyeon Yang, Xiaodong Mu, Ioulia B. Zotova, Yujie J. Ding, and Gregory J. Salamo, Physics Department, University of Arkansas, Fayetteville, AR.

We report a study on self-assembled InAs quantum wires (QWR) on a planar surface of InP(001), grown by molecular beam epitaxy and examined by in situ scanning tunneling microscopy and photoluminescence (PL). The detailed morphology of the quantum wires including width and height distributions and its correlation with PL data will be presented. Correlation of morphology with PL intensity suggests that the PL peak is due to a wire size of 36 nm^2. The spectral range of the PL emission from the QWR includes the technologically important 1.55 μm and the PL emission peak shows a temperature sensitivity of 0.17nm/°C. High optical polarization anisotropy of more than 50% from the quantum wires has been observed at room temperature and at 4.2K over a wide range of PL emission wavelength, indicating that a majority of quantum wires of various heights and widths participate in strong carrier confinement.

SESSION N7: QUANTUM DOTS—APPLICATIONS AND PROPERTIES
Chairs: Robert Hull and Gregory L. Snider
Wednesday Afternoon, November 28, 2001
Room 306 (Hynes)

1:30 PM *N7.1
1D-STACKING OF STRAINED QUANTUM DOTS VIA SELF-ORGANIZATION AND DURING WHISKER GROWTH. Lars Samuelson, Lund University, Solid State Physics/Nanometer Consortium, Lund, SWEDEN.

Internally arranged quantum dots forming 1-dimensional stacks of coupled quantum dots, or super-lattices of quantum dots, are of great interest for future applications in quantum devices, for quantum computing and for THz-emitting Bloch oscillators. I will in this talk discuss two approaches that we have developed in this area of quantum materials research. The first example is from the use of Stranski-Krastanow grown quantum dots, in which the strain field distribution from a first layer of QDs can be used to self-organize a second (and third) layer of quantum dots, reproducing the position of the QDs formed in the first layer. We have recently been able to incorporate such stacks of quantum dots as active elements in resonant tunneling diodes, in which double layers of InAs SK-growth QDs are placed in-between barriers of InP, having GaInAs as emitter and collector regions. Such RT-devices have shown exceptionally sharp IV-features, including peak-to-valley ratios of as high as 85, reflecting the resonant coupling between two totally quantized zero-dimensional objects. The second example to be discussed is the formation of non-lattice-matched layers inside nano-whiskers grown by the vapor-liquid-solid (VLS) growth mode. This is based on the formation of a eutectic alloy of Au and In, from which whiskers of e.g. InAs and InP are formed with the diameter of the nano-whisker governed by the diameter of the supplied catalytic nano-particle. Finally I will show that abrupt hetero-interfaces of non-lattice-matched InAs-InP combinations can be formed inside these nano-whiskers, resulting in controlled formation of strained hetero-barriers as well as strained quantum dots inside a nano-whisker.

2:00 PM N7.2
3D HEXAGONAL ORDERING IN VERTICALLY ALIGNED PbSe QUANTUM DOT SUPERLATTICES. A. Raab, R.T. Lechner, G. Springholz Johannes Kepler Universitaet, Linz, AUSTRIA.

Self-organization during the growth of quantum dot superlattices has been shown to result in the formation of different types of vertically and laterally ordered dot superstructures. In particular, for self-assembled PbSe/PbEuTe quantum dot superlattices either an fcc-like dot stacking or a vertical dot alignment may be formed, depending on the spacer thickness inserted between the dot layers (1). For the fcc-stacked superlattices, the highly efficient ordering process has been demonstrated in our previous work (2). Here we investigate the lateral ordering process for the case of vertically aligned PbSe dot superlattices that occurs when the spacer layer thicknesses is less than 30 nm. From atomic force microscopy studies it is shown that the most pronounced in-plane ordering takes place when the spacer thickness is around 15 nm. High resolution x-ray diffraction reciprocal space maps show that due to the alignment of the dots along the growth direction, a 3D hexagonal dot arrangement is formed with a very pronounced narrowing of the dot size distribution. In addition, an increase of the lateral dot separations with increasing vertical superlattice period is found. As is shown by strain calculations as well as growth simulations, the lateral ordering tendency for the vertically aligned dot superlattices is explained by elastic repulsion between next-nearest neighboring dots in adjacent dot layers rather than by elastic attraction as is the case for the dot superlattices with fcc-stacking. (1) G. Springholz, et al., Phys. Rev. Lett. 84, 4669 (2000). (2) M. Pinczolits, et al., Phys. Rev. B 60, 11524 (1999).

2:15 PM N7.3
CHARACTERIZATION OF THE VERTICAL-ANTICORRELATION ARRAYS OF InAs/InAlAs NANOWIRES WITH A FIXED LAYER-ORDERING ORIENTATION. Zhongzhe Sun, Soon Fatt Yoon, School of Electrical and Electronic Engineering, Nanyang Technological University, REPUBLIC OF SINGAPORE; Zhanguo Wang, Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, Beijing, PEOPLE'S REPUBLIC OF CHINA.

The InAs/InAlAs nanowire multilayer arrays on (001) InP were found to exhibit specific spatial ordering. Regardless of the change in the InAlAs spacer thickness of different samples, (i) the nanowires of one InAs layer are positioned above the spacing of nanowires in the previous InAs layer and (ii) the layer-ordering orientation of nanowires is fixed. Transmission electron microscopy study reveals that such an array is just the stable self-consistent structure of the InAs/InAlAs multilayer dynamic system. The inherent tendencies of the system, that the surface of the InAlAs spacer layer tends to follow the morphology of the InAs layer underneath and that the strain-induced composition and thickness modulations of the InAlAs spacer layer favor a wavelength proportional to its thickness, establish the characteristics of the nanowire array.

2:30 PM N7.4
STRUCTURAL AND OPTICAL CHARACTERISATION OF STACKED SELF-ASSEMBLED InAs/GaAs QDs. Peter B. Joyce, Tomasz J. Krzyzewski, Jim H. Neave, Gavin R. Bell, Tim S. Jones, Centre for Electronic Materials and Devices and Department of Chemistry, Imperial College, London, UNITED KINGDOM; Eric C. Le Ru, Ray Murray, Centre for Electronic Materials and Devices and Department of Physics, Imperial College, London, UNITED KINGDOM.

The growth of InAs quantum dots (QDs) on GaAs(001) substrates has been the focus of a large amount of research activity due to their potential for producing lasers with a low, temperature independent threshold current. We have previously shown that it is possible to achieve 1.3 μm room temperature emission by growing at low InAs deposition rates. However, the gain from a single QD layer is not sufficient for laser applications and multiple QD layers are necessary. We present a detailed study on the effect of the GaAs spacer layer thickness on the properties of InAs/GaAs QDs grown on GaAs(001) substrates by molecular beam epitaxy (MBE). Reflection high energy electron diffraction (RHEED) measurements show that for thin GaAs spacers ($<200\AA$) there is a reduction in the critical thickness (θ_{crit}) for the 2D to 3D growth mode transition. Scanning tunnelling microscopy (STM) measurements of uncapped QDs reveal that the QDs in the first and second layer separated by $420\AA$ of GaAs have the same average volume and similar number density. By contrast, when a thin spacer layer is used ($120\AA$) the number density of the QDs in the second layer is a factor of two less than in the first layer. The average volume of the QDs in the second layer is also considerably larger than in the first layer. Photoluminescence (PL) measurements of capped bilayer QD samples show that the emission from a QD sample separated by $420\AA$ GaAs results in a single peak, whereas separation by $120\AA$ results in two emission peaks which can be made coincident by tuning the amount of InAs deposited in the second layer. The results can be rationalised by the different growth mechanisms in the two layers since the morphological template for second layer QD growth is very different to first layer growth.

2:45 PM N7.5
OPTICAL CHARACTERIZATION OF SELF-ASSEMBLED Ge DOTS ON SILICON. F. Marabelli[a], A. Rastelli[a,b], A. Valsesia[a], H. von Känel[b], [a]INFM-Phys. Dept."A. Volta", University of Pavia, ITALY; [b]Laboratorium für Festkörperphysik, ETH Zürich, SWITZERLAND.

Self assembled quantum dots of Ge were obtained by magnetron sputter epitaxy of seven monolayers of Ge on a 33nm thick undoped Si buffer grown on top of a p-doped (100) Si substrate. The samples obtained in this manner were then capped with an increasing number of silicon layers in order to study the effect of Si deposition on the strain and the morphology of the dots. The shape evolution of the dots was studied by UHV scanning tunneling microscopy (STM). They were then characterized "ex situ" by spectroscopic ellipsometry, reflectance and Raman spectroscopy. The optical experiments revealed well defined differences between the capped and uncapped samples and among samples with different cap thicknesses. By monitoring the energy and the splitting of the E0, E1 and E2 interband optical transitions of Ge and by measuring the Ge-Ge and Ge-Si vibrational modes, the optical measurements evidence strain effects as well as the formation of SiGe alloy, in agreement with the "in situ" STM measurements.

3:30 PM *N7.6
QUANTUM-DOT CELLULAR AUTOMATA: DEVICES AND ISSUES. Gregory L. Snider, Univ. of Notre Dame, Dept. of Electrical Engineering, Notre Dame, IN.

For over 30 years the microelectronics industry has enjoyed dramatic improvements in the speed and size of electronic devices. This trend has long obeyed Moore's law, which predicts that the number of devices integrated on a chip will double every 18 months. Adherence to this exponential growth curve has been a monumental task requiring rapid improvements in all aspects of integrated circuit (IC) fabrication. At some point in the future, a follow-on technology will be needed, as further scaling of CMOS becomes impossible. Quantum-dot Cellular Automata (QCA) is a revolutionary architecture employing quantum dots for digital computation, and holds the promise of high device density and low power dissipation, beyond that possible in CMOS. A basic QCA cell consists of four quantum dots located at the corners of a square, coupled capacitively and by tunnel barriers. The cell is biased to contain two excess electrons within the four dots, which are forced to opposite "corners" of the four-dot cell by mutual Coulomb repulsion. These two possible polarization states of the cell are used to represent logic "0" and "1". Properly arranged, arrays of these basic cells can implement Boolean logic functions. In this presentation, an introduction to the QCA architecture will be given along with experimental results from the first demonstrations of QCA devices using aluminum islands as the dots. In addition, other possible QCA implementations will be discussed, including molecules and semiconductor dots.

4:00 PM N7.7
SCANNING TUNNELING MICROSCOPY INVESTIGATION OF GaAa/GaP SELF-ASSEMBLED ISLANDS. P. Ballet, H. Yang, C.L. Workman, Z.M. Wang, W.Q. Ma and G.J. Salamo, Physics Department, University of Arkansas, Fayetteville, AR.

We present a scanning tunneling microscope investigation of the morphology of GaAs/GaP three-dimensional (3D) islands obtained by molecular beam epitaxy. These quantum structures have a potentially valuable spectrum covering the red and yellow regions. In addition, the fact that this system is Ga-based leads to higher growth temperatures compared to the In-based systems, typically 580C instead of 500C. This is of technological importance because all systems utilizing In for the generation of strain undergo significant change in their optical properties when the growth temperature is brought to 600C and above for the growth of the Al-based cladding layers necessary to fabricate efficient light emitting device. The islands are found in the form of self-assembled wires along [-110]. The facets are oriented toward [-113] or [-112] depending on the deposition. The physical origin of the wires is discussed in terms of thin film instabilities in the presence of strain and composition modulations.

4:15 PM N7.8
NEAR-FIELD SCANNING OPTICAL MICROSCOPY INVESTIGATION OF IMMISCIBILITY EFFECTS IN $In_{1-x}Ga_xP$ FILMS GROWN BY LIQUID PHASE EPITAXY. C.A. Paulson, A.B. Ellis, Department of Chemistry, The University of Wisconsin, Madison, WI; P.D. Moran, and T.F. Kuech, Department of Chemical Engineering, The University of Wisconsin, Madison, WI.

We have used Near-field Scanning Optical Microscopy (NSOM) and Electron Probe Microanalysis (EPMA) to study the topographic and microscopic optical properties of several indium gallium phosphide ($In_{1-x}Ga_xP$) samples, with a range of gallium atomic percentages (x), grown by Liquid Phase Epitaxy (LPE) on gallium arsenide (GaAs) substrates. The samples investigated had ~0, 1, and 2 percent lattice-mismatch to the GaAs substrate. NSOM imaging identified strong and highly localized variations in the photoluminescence (PL) intensity and PL peak energy position for films that were highly lattice mismatched with the substrate. The topographic and optical features were highly correlated for these samples. Shifts in the PL peak energy position, by as much as 27 meV, were found during scans across highly mismatched samples, whereas no shifts were seen for ($In_{1-x}Ga_xP$) films with a nearly lattice-matched composition. Both strain and compositional fluctuations could lead to differences in the PL from these samples. X-ray diffraction indicates that these samples were almost completely relaxed hence ruling out strain as the origin of the PL wavelength shifts. Local compositional fluctuations are determined therefore in these measurements. Electron microprobe measurements confirm the local compositional fluctuations albeit on a longer length scale. The NSOM images recorded features that were about 200 nm in their minimum dimension, while the EPMA measurements show features that are a few microns in their minimum dimension. These compositional fluctuations are roughly correlated with the sample topography. These composition fluctuations arise from the solid-solid miscibility gap in the ($In_{1-x}Ga_xP$) system at the growth temperatures. These results illustrate how NSOM can be used as a high spatial resolution probe of phase segregation effects on the materials properties of a broad class of light-emitting semiconductor alloys possessing miscibility gaps.

4:30 PM N7.9
OBSERVATIONS OF AlN THIN FILM GROWTH ON SAPPHIRE AND III-NITRIDE SUBSTRATES BY MBE. Mark Yeadon, IMRE and Dept of Materials Science, National University of Singapore, SINGAPORE; Xu Zhang, Kian Ping Loh, Dept of Chemistry, National University of Singapore, SINGAPORE; Eric Stach, NCEM, Lawrence Berkeley National Laboratory, Berkeley, CA.

The novel electronic and optoelectronic properties of III-nitride compounds (including BN, AlN, GaN and InN) have inspired intense activity in the development of device quality thin films of these materials. In recent years, reliable blue and UV-emitting GaN LEDs have become commercially available. Our understanding of the fundamental mechanisms of defect introduction and propagation in these materials is still very limited, however. Our experiments focus on understanding the underlying mechanisms governing the microstructure and physical properties of epitaxial III-nitride thin films. Using an UHV transmission electron microscope (JEOL JEM 2000V) with in-situ MBE capability, we are investigating the growth of AlN thin films on a variety of substrates including sapphire and GaN. In this paper we present the results of our study and evidence for strain-induced island formation during AlN formation on the sapphire surface.

4:45 PM N7.10
InAs QUANTUM DOTS FORMATION, EVOLUTION AND EVAPORATION ON GaAs AND AlAs SURFACES. M. Yakimov, V. Tokranov, A. Katsnelson and S. Oktyabrsky, U Albany Institute for Materials, University at Albany-SUNY, Albany, NY.

We have studied the kinetics of formation and evaporation of InAs quantum dots (QDs) grown by molecular beam epitaxy on GaAs(100) surface and thin (submonolayers to 2 ML) AlAs layers in a temperature range from 350°C to 550°C. In-situ reflection high energy electron diffraction (RHEED) patterns were recorded in real time and analyzed to reveal the 2D-3D transition in the RHEED pattern, indicating the QD formation, consequent ripening process and evaporation of the QDs at higher temperatures. Experiments were performed at In fluxes corresponding to 0.045 and 0.45 ML/s, and constant As_2 overpressure, 10^{-6} Torr measured by beam flux monitor. Intensity distribution in RHEED pattern was measured either by a single photodiode for high dynamic range measurement or recorded by a CCD camera with consequent analysis of intensity distribution and streaking in different areas of the pattern. As the InAs coverage was increasing, the RHEED pattern was found to evolve from weak 2D streaks for under-critical InAs coverage corresponding to a rough wetting layer, to well-defined chevron-shaped spots along [01-1] zone for the just formed small facetted QDs. During the consequent ripening process chevron shape became less defined, indicating redistribution of InAs toward the larger QDs. At higher temperatures (> 475°C), the exposure of the InAs-covered surface resulted in the streaky diffraction pattern due to the evaporation of the In atoms. The observed peculiarities in the In evaporation behavior from GaAs and AlAs surfaces were attributed to different rates of In intermixing with the underlayers. The obtained data on In evaporation were used to explain the high temperature behavior of the critical thickness and dynamics of QD formation.

SESSION N8: RELAXATION, MORPHOLOGY AND COMPOSITION MODULATIONS
Chairs: Joanna Mirecki-Millunchick and Rosa Leon
Thursday Morning, November 29, 2001
Room 306 (Hynes)

8:30 AM *N8.1
EFFECTS OF DISLOCATIONS IN STRANSKI-KRASTANOW QUANTUM DOTS. Rosa Leon, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA.

The interrelations between structural and optical properties in Stranski-Krastanow (S-K) quantum dots are examined trough different experiments that explore III-V quantum dots (QD) formation. First, the evolution of ternary InGaAs QDs using a positionally varying growth rate will be described. Island densities were seen to increase exponentially before saturation. Photoluminescence (PL) of capped structures showed that wetting layer (WL) PL energies did not shift beyond the onset of the S-K transition. After saturation, a sharp drop in PL intensity was observed, which was attributed to island coalescence and incoherent island formation. In a multilayered InGaAs/GaAs quantum-dot (QD) structure, a transition between two types of step alignment, and a change to larger QD sizes in smaller concentrations was observed after formation of a dislocation array. Cathodoluminescence (CL) spectra showed a bimodal peak with lower energy peak enhancement when probing at lower e- beam energies. CL imaging and cross-sectional transmission electron microscopy showed contrast from a dislocation array formed at the interface between GaAs and the first InGaAs QD layer. Strong QD emission in the near infrared (800 to 1100 nm) was obtained despite the presence of dislocations. Highly ordered patterns of InAs QDs were obtained on InGaAs dislocation arrays, where rectangular patterns of misfit dislocations are transferred into well-separated rows of sharply aligned InAs quantum dots. Since dislocations may act as nonradiative recombination centers and reduce QD carrier lifetimes, their optical properties were compared with those of standard InAs QD structures. The most striking difference observed was in the dependence of the PL intensity on photoexcitation power. Without dislocations, the PL intensity increases linearly with excitation intensity, indicating that efficiency of carrier transfer from the barriers into the dots is not carrier-density dependent. On the other hand, dependence of the QD PL intensity on excitation intensity exhibits a strongly superlinear behavior in the ordered QD samples. This effect is attributed to carrier trapping at the dislocation layer, which reduces the number of carriers reaching the QDs.

9:00 AM N8.2
SIZE EFFECTS AND SCALING IN MISFIT DISLOCATION FORMATION IN SELF ASSEMBLED QUAUNTUM DOTS. Lawrence H. Friedman, Netherlands Institute for Metals Research, TU Delft, Delft, THE NETHERLANDS; Daniel M. Weygand and Erik van der Giessen, Netherlands Institute for Metals Research, University of Groningen, Groningen, THE NETHERLANDS.

Stranski-Krastanow (SK) growth can be used to produce large arrays of quantum dots. An important aspect of SK growth is lattice misfit strain relaxation by the formation of misfit dislocations. Johnson and Freund (J. Appl. Phys. 81(9), 1997, p6081) developed a 2D model of misfit dislocation nucleation in SK growth islands whereby they predict a powerlaw relation between misfit strain, ϵ_m, and the minimum island size to nucleate a misfit dislocation, R: $\epsilon_m = AR^{\lambda-1}$, where λ is a function of the island-substrate contact angle, which is solvable from the linear elastic theory of wedges. Friedman, Weygand and Van der Giessen (MRS Spring 2001 Meeting, Symposium P: "Dislocations and Deformation Mechanisms in Thin Films and Small Structures") have proposed how a nodal model of 3D dislocation dynamics can be adapted to extend the model of Johnson and Freund to 3D. Like the 2D model, the 3D model is based on the linear elastic theory of dislocations. Misfit dislocation formation is controlled by balancing misfit strain relaxation with "image forces" which hinder the formation of misfit dislocations. Both of these effects are incorporated via the Finite Element Method. The applicability of the powerlaw of Johnson and Freund is discussed in light of the 3D model results. The model itself is discussed as a step towards more general modeling of dislocations in complex heterogeneous environments. (The authors gratefully acknowledge funding from The Netherlands Institute for Metals Research, project MS97006B.)

9:15 AM N8.3
SiGe EPILAYER STRESS RELAXATION: QUANTITATIVE RELATIONSHIPS BETWEEN EVOLUTION OF SURFACE MORPHOLOGY AND MISFIT DISLOCATION ARRAYS. Jennifer Gray, Robert Hull, Univ of Virginia, Dept of Materials

Science and Engineering, Charlottesville, VA; Jerry Floro, Sandia National Laboratories, Albuquerque, NM.

The kinetics of stress relaxation have been measured in real time using in situ wafer curvature measurements during SiGe/Si heteroepitaxial growth. This real-time data has been combined with detailed analysis of the evolving surface morphology and misfit dislocation density using atomic force microscopy and transmission electron microscopy. SiGe thin films were grown on Si (001) substrates in a molecular beam epitaxy chamber equipped with reflection high energy electron diffraction and an in-situ multi-beam optical stress sensor system to monitor stress relaxation. Several distinct stages of microstructural evolution were observed during epitaxial growth of $Ge_{0.3}Si_{0.7}$ alloys at 550°C. Initial planar, coherent growth was followed by the development of an unusual island morphology at layer thicknesses on the order of 20nm. This island morphology consists of square islands with walls oriented along the < 100 > directions enclosing pits in what may be a cooperative nucleation process. Dislocations are next introduced into the film abruptly at 50nm film thickness and rapidly relieve the stress so that approximately 90% relaxation is seen after subsequent 50nm of growth. The surface morphology of the film after dislocation introduction consists of cross-hatch trenches aligned along the < 110 > directions. As the dislocation density increases in the film, the coherent island/pit structures begin to disappear and the film morphology is dominated by the evolving cross-hatch morphology. The effect of changing growth rate and temperature on this surface morphology and subsequent dislocation formation will also be reported. Implications for competitive and/or correlated relaxation of strain by misfit dislocations and surface morphology based upon this data will be discussed. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.

9:30 AM N8.4
THE STRAIN RELAXATION MECHANISM IN Ge(Si)/Si QUANTUM DOTS GROWN AT HIGH-TEMPERATURES. Jin Zou, Xiaozhou Liao, the University of Sydney, Australian Key Center for Microscopy & Microanalysis, NSW, AUSTRALIA; David J.H. Cockayne, University of Oxford, Department of Materials, Oxford, UNITED KINGDOM; Zuimin Jiang, Xun Wang, Fudan University, Surface Physics Laboratory, CHINA.

The growth and strain relaxation of semiconductor quantum dots have been paid enormous attention. In particular, self-assembled Ge islands grown on Si surfaces have been well investigated in many aspects. However, little study has been carried out to understand the formation mechanism of misfit dislocations in this system at higher growth temperatures. In this work, we use transmission electron microscopy to study the core structures of misfit dislocations in Ge(Si)/Si(001) islands grown by solid-source molecular beam epitaxy at a high temperature of 700°C. Cross-section investigation shows different misfit dislocation morphology, namely, Lomer misfit dislocations, 60° perfect dislocations and 30° partial dislocations associated with stacking faults. The distances between these misfit dislocations within an island and the dislocations morphologies suggest that the dislocations are not generated from the island edge at the island/substrate interface but from the island surface above the interface. Elasticity theory calculation also conforms this strain relaxation mechanism.

9:45 AM N8.5
QUANTUM DOTS WITH HETEROSTRUCTURAL WETTING LAYERS. P. Finnie, B. Riel[a], G. Aers, S. Raymond, C. Allen[a], Z. Wasilewski, National Research Council Canada, Ottawa, CANADA. [a]also with Dept of Physics, Univ of Ottawa, Ottawa, CANADA.

The archetypal system for self-assembled quantum dot formation is InAs on GaAs, which grows in the Stranski-Krastanov (SK) mode: the first ~2 ML of InAs adjust to the GaAs lattice constant, forming a two-dimensional film of InAs. Above this critical thickness, minuscule three-dimensional "quantum dot" islands are formed. Many materials grow in the SK mode while many other materials grow in the Volmer-Weber (VW) mode, in which islands form without the two-dimensional "wetting layer" film. In the more general situation, the layer beneath the dots need not be homogeneous. The dynamics of SK dot nucleation is explored for molecular beam epitaxy in the case that the wetting layer itself is a vertical heterostructure. The rules for quantum dot nucleation on simple wetting layer heterostructures are determined experimentally using in situ reflection high-energy electron diffraction. This type of growth procedure creates a number of often-neglected opportunities. As an extreme case, a material that ordinarily grows in the SK mode can be made to grow without a true wetting layer ("pseudo-VW growth"). Likewise, a material that ordinary grows in the VW mode may potentially be forced to grow with a "wetting layer" ("pseudo-SK growth"). The presence or absence of a wetting layer becomes, in a sense, optional.

10:30 AM N8.6
COMPOSITION DISTRIBUTION OF AS-GROWN AND ANNEALED Ge(Si)/Si(001) ISLANDS. Xiaozhou Liao, Los Alamos National Laboratory, Division of Materials Science and Technology, NM; Jin Zou, University of Sydney, Australian Key Center for Microscopy & Microanalysis, NSW, AUSTRALIA; David J.H. Cockayne, University of Oxford, Department of Materials, Oxford, UNITED KINGDOM; Jun Wan, Zuimin Jiang, Gaolong Jin, and Kang L. Wang, University of California at Los Angeles, Electrical Engineering Department, Los Angeles, CA.

Ge(Si)/Si(001) multi-layer islands produced by gas-source molecular beam epitaxy at 575°C were investigated using cross-section energy-filtering transmission electron microscopy and X-ray energy dispersive spectrometry. Investigation of as-grown on the top unburied islands with a large magnification shows non-uniform composition distribution in the islands with a suggestion that the highest Ge content is at the island center. The average Ge content in the islands is much higher than in the wetting layer. The island/substrate and the wetting layer/substrate interfaces have been moved to the substrate side. A growth mechanism of the islands, which includes alloying, elemental enrichment and interdiffusion processes, is discussed based on the composition distribution and the interfacial structures. Results in a lower magnification (and therefore a larger area) show, for as-grown samples, not only a continuous enlargement of island size in upper layers but also a continuous increase of Ge concentration within islands in upper layers. As a result of the increasing island size and Ge concentration within the islands, the island density decreases in upper layers. For samples annealed at 900°C for five minutes, the aspect ratio of buried islands increases significantly and the average Ge concentration within islands of different layers becomes uniform.

10:45 AM N8.7
NANOMETER-SCALE STUDIES OF PHASE SEPARATION IN MISFIT-FREE InAlAs SEMICONDUCTOR ALLOYS. B. Shin, A. Lin, K. Lappo, and R.S. Goldman, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI; M.C. Hanna, S. Francoeur, A.G. Norman, and A. Mascarenhas, National Renewable Energy Laboratory, Golden, CO.

In recent years, compound semiconductor alloys have been incorporated into a range of electronic and optoelectronic devices. In most of these systems, growth conditions have been reported for which phase separation occurs. Yet, the thermodynamic versus kinetic origin of phase separation, as well as the experimental conditions for determining the presence of phase separation has been the subject of debate for nearly twenty years [1, 2]. In thin films of compound semiconductor alloys, both the difference in binary bond lengths and the film/substrate misfit are expected to play a significant role in the initiation of alloy phase separation. In this work, we have examined phase separation in the misfit-free InAlAs/InP system using ultra-high vacuum cross-sectional scanning tunneling microscopy (XSTM) and x-ray reciprocal space mapping. XSTM reveals isotropic nanometer sized clusters in p-doped InAlAs films. For thicker, undoped InAlAs layers, longer wavelength quasi-periodic modulations perpendicular to the growth direction are apparent. Interestingly, the average modulation wavelength increases with film thickness, reaching a saturation value at ~25nm thickness. This value is consistent with the modulation wavelength determined from (002) x-ray reciprocal space maps, suggesting that the lateral modulations are primarily due to composition variations. In addition, these modulation wavelengths are notably lower than those reported for similar films grown at higher temperatures [3]. Together, these results suggest that lateral phase separation in this system is a thermally activated kinetic process, which may be affected by the presence of impurities such as dopants. [1] G.B. Stringfellow, J. Cryst. Growth 65, 454 (1983). [2] A. Zunger and S. Mahajan, in Handbook on Semiconductors (North-Holland, Amsterdam, 1994), Vol. 3, p1399. [3] H.K. Cho et al, Mat. Sci. Eng. B64, 174 (1999).

11:00 AM N8.8
ATOMIC SELF-ORDERING IN ORDINARILY STRAINED SEMICONDUCTOR QUANTUM DOTS AS A CONSEQUENCE OF INTERACTIONS BETWEEN INTERNAL AND EXTERNAL STRAINS. P. Möck, T. Topuria, Y.Y. Lei, D. Browning, Department of Physics, University of Illinois at Chicago, Chicago, IL.

Self-assembled ordinarily strained quantum dots (OS-QDs) can be produced in many binary element and pseudo-binary compound semiconductor systems by heteroepitaxial growth in the Stranski-Krastanow mode. In addition to the well known self-ordering of OS-QDs on a tens of nm scale, self-ordering on the atomic length scale has recently been observed by means of transmission electron microscopy in both the scanning probe Z-contrast[1,2] and parallel illumination[2,3] modes. Such self-ordering on the atomic length scale leads to novel type quantum dots[2] (ICM-QDs), that are characterized

by internal compositional modulations (ICMs). These ICMs are discussed in this paper to arise from interactions between internal strains (due to different bonds lengths and angles between the constituent atoms) and external strains (due to lattice mismatch between OS-QDs and their surrounding matrix). As ICM-QDs have already been observed in several semiconductor quantum dot systems and for the transformation of OS-QDs into ICM-QDs seems to be thermodynamically favored in general, we suspect that only the latter are structurally stable over the lifetime of possible opto-electronic devices. Controlling the interaction between internal and external strains and thermal treatments in a certain temperature range, on the other hand, may open a route towards the production of nano-sized semiconductor agglomerates with novel structures.

[1]P. Möck et al, J. Electron. Mater, June 2001 special topic issue on II-VI compound semiconductors.
[2]P. Möck et al., in press Appl. Phys. Lett.
[3]P. Werner et al, Proc. 6^{th} International Symposium on Advanced Physical Fields, Growth of Well defined Nano-structures, Tsukuba, March 6^{th} - 10^{th}, 2001, p. 132.

11:15 AM N8.9
COMPOSITIONALLY MODULATED STRUCTURES STUDIED BY IN SITU SCANNING TUNNELING MICROSCOPY. C.A. Pearson, Department of Computer Science, Engineering Science and Physics, University of Michigan-Flint, Flint, MI; C. Dorin, J. Mirecki Millunchick, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI; Y. Chen, B.G. Orr, Department of Physics, University of Michigan, Ann Arbor, MI.

Two different short period superlattice (SPS) structures with nominally equivalent lattice mismatch, AlAs/InAs and GaAs/InAs are examined using in situ scanning tunneling microscopy (STM). Depending upon the growth conditions, the composition of the AlAs/InAs SPS structure can be either homogeneous or modulated in the lateral direction. The compositional difference is immediately apparent in STM images of the SPS surface. Distinct periodic structures are clearly visible in images of the modulated SPS while no periodicity is observed in the homogeneous SPS. For a 30 period SPS of 2 ML of AlAs and 2 ML of InAs we observe structures 20 nm in size with an average spacing of 30 nm in orthogonal directions. Despite the nominally equivalent lattice mismatch, the GaAs/InAs SPS structures are quite different. Some degree of modulation is always observed in these structures. Homogeneous structures are not observed. For the modulated SPS structures, chemical profile is characterized using scanning tunneling spectroscopy. Results are compared to a kinetic model incorporating In segregation.

11:30 AM N8.10
MIXING THERMODYNAMICS OF BINARY-ALLOY FILMS COHERENT WITH FROZEN COMPOSITIONAL PERTURBATIONS. Stephen Lee, Sandia National Labs, Albquerque, NM.

Several previous studies have examined the growth of binary alloys by using linear instability theory to analyze time-dependent surface diffusion and deposition. In these models, coherent epitaxy of mobile binary-alloy monolayers occurs upon a lateral compositional perturbation wave that is "frozen" into the near-surface region of a crystal. For a special case, lattice-matched planar growth where the binary-alloy components have different lattice constants, they find that binary alloys can become unstable at a critical temperature far above the bulk chemical spinodal. We determine the thermodynamic ground-state of the same physical system, but in the absence of growth. The thermodynamic approach clarifies the elastic mechanism that underpins the enhanced instability. Several key results are obtained: (1) decomposition of the mobile overlayer at temperatures above the chemical spinodal results from minimizing the free-energy of the restricted thermodynamic system defined by initial assumptions – a very thin and mobile binary-alloy film lies coherently upon a perfectly immobile compositional perturbation; these assumptions and not dynamical processes produce the basic instability, (2) the strain field at the free surface of the perturbation creates elastic energy in the coherently strained epitaxial overlayer where none would ordinarily exist thereby raising the total energy; lateral variation of this elastic energy alone alters the critical temperature and induces compositional fluctuations at restricted equilibrium; (3) since the strain field of the perturbation is geometry dependent, the perturbed critical temperature is also geometry dependent; linear-instability analyses give the maximum critical temperature; (4) this maximum occurs when the thickness of the perturbation exceeds the lateral wavelength of the perturbation; (5) consequently, in the early stage of film growth only very short wavelength decomposition is enabled by this instability. The U.S. Dept. of Energy, Office of Basic Energy Sciences, supports this work.

11:45 AM N8.11
THE FORMATION OF SELF-ASSEMBLED Cu_2O NANOSTRUCTURES INVESTIGATED BY IN-SITU UHV TEM. Guang-wen Zhou, Judith C. Yang, University of Pittsburgh, Dept. of Materials Science and Engineering, Pittsburgh, PA.

There is a considerable interest in understanding the exact formation process of self-assembled nanometer scale islands in strained materials both from a fundamental, as well as an application point of view. Currently, various techniques are used to grow self-organized epitaxial nanostructures on substrates with different lattice constants. In this work, we chose Cu as a model system to demonstrate an approach to grow oxide nanostructures through self-assembly process by oxidizing Cu films within an in-situ UHV TEM. In situ oxidation also provides fundamental information on the initial oxidation kinetics. It has shown that the structure, morphology, size, and distribution of the oxide nanostructure can be monitored by controlling the oxidation conditions. The microscope used for this experiment is a modified JEOL200CX, an attached leak valve to the column of the microscope permits the introduction of gases directly into the microscope. A UHV chamber was attached to the middle of the column, where the base pressure is less than 10^{-8}Torr. Single crystal 99.999% pure Cu(100), (110), and (111) films were grown on in an UHV e-beam evaporator system, where the base pressure was 10^{-10} torr. The Cu films were oxidized in situ between temperature ranging from room temperature to 1000°C and oxygen pressure ranging from 5×10^{-4} torr to 760 torr. The formation, morphology evolution, and coalescence of Cu_2O islands as a function of oxidation conditions, i.e. substrate orientation, oxidation temperature, oxidation time, and oxygen pressure were investigated in situ. SEM, AFM and HREM were used to investigate the surface topology and the microstructures of these self-assembled oxide nanostructures. The oxide nano-structures were also obtained by in-situ oxidizing Ti and Co systems.

SESSION N9: HETEROEPITAXY IN METALS AND OXIDES
Chairs: Ivan K. Schuller and Dongqi Li
Thursday Afternoon, November 29, 2001
Room 306 (Hynes)

1:30 PM *N9.1
SELF-ASSEMBLED MAGNETIC DOTS, ANTIDOTS, DOT CHAINS, AND STRIPES: EPITAXIAL COBALT ON Ru(0001). Dongqi Li, Materials Science Division, Argonne National Laboratory, Argonne, IL.

Magnetic nanostructures are of great interest for both fundamental scientific research and technological development. At the forefront of the field is the fabrication of lateral structures via self-assembly techniques. Recently, we have observed a novel metal-on-metal growth mode for Co grown via MBE onto Ru(0001). We find that three-dimensional Co islands (dots) or a flat Co film network with deep holes (antidots) in truncated pyramidal shapes exist, as characterized by means of ex-situ AFM.[1] The tops of the islands and the rims of the holes are virtually atomically flat. The lateral sizes of these dots/antidots, $\sim 10^2$ nm, tend to be uniform. We postulate that this growth mode, similar to that of self-assembled quantum dots in semiconductors, is mainly driven by strain due to lateral mismatch between the basil plane lattice constants of bulk Co and Ru. These dots are ferromagnetic with in-plane, single magnetic domains in their virgin state. While the self-assembled structures are intrinsically simple to produce and have the potential to reach beyond the limitations of lithographic length-scales, a barrier for potential applications is the difficulty in positioning the nanostructures in desired locations. We have explored the placement of these dots on a grooved Ru(0001) surface. The dots automatically align into linear chains along the asymmetric grooves to form either dot chains or continuous stripes. There is evidence that diffusion, in addition to strain, may also play a role in the nucleation of these dots. It becomes promising that such dot alignment can be achieved via lithographically assisted self-assembly. This would open new opportunities by creating templates and scaffolds for the growth of either ordered magnetic arrays or arbitrary arrangements.
Work supported by the US DOE BES-Materials Sciences under contract #W-31-109-ENG-38.
1. Chengtao Yu, Dongqi Li, J. Pearson, and S.D. Bader, Appl. Phys. Lett. 78, 1228 (2001).

2:00 PM N9.2
FIRST-PRINCIPLES THEORY OF ELASTIC RELAXATIONS AND NANOSCALE ORDERING IN ULTRATHIN ALLOY FILMS. Vidvuds Ozolins, Sandia National Labs, Dept of Thin Film and Interface Science, Livermore, CA; Mark Asta, Northwestern Univ, Dept of Materials Science and Engineering, Evanston, IL; J.J. Hoyt, Sandia National Labs, Dept of Materials & Process Modeling, Albuquerque, NM.

Recently a growing number of experimental observations have reported the spontaneous formation of nano-scale domain structures on morphologically flat crystalline surfaces. The stability of such structures has been qualitatively explained to occur due to the formation of periodic stress domains that act to lower the energy of compositionally inhomogeneous surfaces. We develop a *quantitative atomistic* theory describing the thermodynamic driving force for self-assembly of nano-scale structures in ultrathin alloy films. Specifically, we study a monolayer film of $A_{1-c}B_c$ alloy. Ordering and clustering instabilities in the film are governed by the Fourier transform of the effective pair interactions, $V(\mathbf{k})$. Analytic expressions for $V(\mathbf{k})$ are derived using an atomistic model of surface alloy energetics based upon the well-known Frenkel-Kontorova (FK) scheme in the small-displacement (harmonic) limit. In contrast to the standard FK scheme, substrate relaxations are fully incorporated. The parameters of this model have a simple physical interpretation and are obtained entirely *ab initio* using first-principles electronic-structure calculations. Sucessful applications to first-principles studies of nanoscale laterally composition-modulated structures in $Co_{1-x}Ag_x$ on Ru(0001) are demonstrated.

2:15 PM N9.3
ATOMISTIC MODELING OF Co GROWTH ON Cu(111). Joseph Khalil, NASA Glenn Research Center, Cleveland, OH; Guillermo Bozzolo, Ohio Aerospace Institute and NASA Glenn Research Center, Cleveland, OH; Daniel Farías, A.L. Vázquez de Parga, J.J. de Miguel, R. Miranda, Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, SPAIN.

Recent experimental analysis of Co growth on Cu(111) has raised interesting questions regarding the low coverage regime and the identification of the driving mechanisms that lead to the observed structures. The understanding of such phenomena would allow for controlling the structure and morphology of the growing films to achieve the desired properties. Some of the observed features include triangular-shaped islands with a height of two layers above the surface, decoration of the Cu step edges with mixed Co and Cu clusters, and monatomic-deep pools of vacancies in the surface [1]. We present preliminary results of a modeling effort based on the BFS method for alloys [2], meant to elucidate the main characteristics of the early growth stages of Co films on Cu(111). Analytical calculations for the determination of the surface structure are supplemented with temperature-dependent Monte Carlo simulations. After testing the validity of the BFS parameterization (done with first-principles methods) by reproducing basic known features of the system, the methodology is applied to the study of multi-layer islands, their shape, composition and orientation, and the analysis of structural features as the recently reported minority presence of stacking faults in tri-layer islands [3]. [1] J. de la Figuera, J.E. Prieto, C. Ocal and R. Miranda, Surf. Sci. 307-309 (1994) 538. [2] G. Bozzolo, R.D. Noebe, J. Ferrante and C. Amador, J. Comput.-Aided Design 6 (1999) 1. [3] A.L. Vázquez de Parga, F.J. García-Vidal and R. Miranda, Phys. Rev. Lett. 85 (2000) 4365.

2:30 PM N9.4
STRESS RELAXATION DURING TWO-DIMENSIONAL PSEUDOMORPHIC EPITAXIAL GROWTH OF METALS. Stéphane Andrieu, Pascal Turban, Lab. de Physique des Matériaux, CNRS/Université H. Poincaré, Nancy, FRANCE; Pierre Müller, Laurent Lapena, Centre de Recherche sur les Mécanismes de la Croissance Cristalline, CNRS/Universités Aix-Marseille II et III, FRANCE.

Massies and Grandjean discovered that the in-plane lattice spacing oscillates during the heteroepitaxal growth of GaAlAs on GaAs [1]. This phenomenon was also found to occur during the epitaxy of metals as reported by Fassbender et al [2] and Turban et al [3]. The physical origin of these oscillations was assumed to be due to the stress relaxation at the 2D islands edges during the growth by birth and spread of these islands. Owing to this possible elastic relaxation, the mean in-plane lattice spacing oscillates from the lattice spacing of the partially relaxed islands towards those of a continuous pseudomorphic layer [4]. First, we explain how the in-plane lattice spacing variations may be deduced from the analysis of RHEED patterns recorded in real time during the growth. The results are analysed for many metallic systems in order to extract pertinent physical parameters, like the misfit and nucleation density. Second, a simulation of what is really measured by using the RHEED technique is proposed. The use of point forces to simulate the surface strain and a semi-dynamical diffraction approach allow us to justify the observations. For example, we show that the amplitude of the in-plane lattice spacing oscillations varies linearly with the misfit and strongly depends on the nucleation density. Thank to this theoretical understanding we discuss experimental results obtained for various metallic systems such as V/Fe(001), Mn/Fe(001), Ni/Fe(001), Co/Cu(001), Fe/Cu(001), Fe/Fe(001), and V/V(001). [1] J. Massies, N. Grandjean, Phys. Rev. Lett. 71, (1993), 1411. [2] J. Fassbender et al, Phys. Rev. Lett. 75, (1995), 4476. [3] P. Turban, L. Hennet, S. Andrieu, Surf. Sci. 446, (2000), 241. [4] R. Kern, P. Müller, Surf. Sci. 392, (1997), 103.

2:45 PM N9.5
SIMULATION OF THE DEPOSITION OF Cu ON (100) Ag AT EXPERIMENTAL DEPOSITION RATES WITH TEMPERATURE ACCELERATED DYNAMICS. J.A. Sprague, F. Montalenti, A.F. Voter, Los Alamos National Laboratory, Theoretical Division, Los Alamos, NM.

The initial stages of growth of (100) Cu films on (100) Ag substrates have been investigated using the temperature accelerated dynamics (TAD) method [1]. Within the accuracy of the harmonic approximation, TAD allows us to boost the system dynamics by several orders of magnitude with respect to standard molecular dynamics while correctly describing the dynamics of all relevant processes. For example, the boost factor for a 0.15-eV process at 77 K is 3×10^8. With this sort of acceleration, it was possible to simulate the deposition of Cu on (100) Ag at 77 K using a deposition rate of 0.04 ML/s, which matched previously reported experiments [2]. These results were achieved without a priori knowledge of the significant atomic processes. For the deposition of Cu on (100) Ag at 77 K, Egelhoff and Jacob [2], observed pseudomorphic growth of the Cu film with persistent RHEED oscillations, indicative of quasi-layer-by-layer growth. The present TAD simulation results showed that the increased lattice parameter of Cu in the film plane reduces the activation energy for the exchange mode of surface diffusion from its value of 0.79 eV for the normal Cu (100) surface to approximately 0.15 eV for the (100) surface of the stretched Cu lattice. This allows the formation of compact Cu islands at 77 K. Furthermore, the TAD simulations revealed some complex mechanisms for Cu atoms to step down from higher to lower terraces in the film.
[1] M.R. Sorensen, and A.F. Voter, J. Chem. Phys. 112, 9599 (2000). [2] W.F. Egelhoff, Jr., and I. Jacob, Phys. Rev. Lett. 62, 921 (1989).

3:30 PM *N9.6
NANOLITHOGRAPHY USING ELECTRON BEAM WRITING AND SELF ASSEMBLY. Ivan K. Schuller, M.I. Montero, O.M. Stoll, Kai Liu and Johan J. Åkerman, Physics Department, University of California-San Diego, La Jolla, CA.

We have used electron beam writing and self assembly to prepare a large variety of Nanostructured Magnetic and Superconducting Arrays. While electron beam writing methods are very flexible, controllable and can produce practically any desired geometry, they are very time consuming and usually the total area that can be covered is very small ($\sim$100 μm x 100 μm). On the other hand, self assembly methods can easily cover macroscopic (1cm x 1 cm) areas and are very fast, however the control over the geometry is much more restricted. I will describe these preparation methods and several physical property measurements where the advantages of each method were exploited. These include the pinning of superconducting vortices by and the hysteresis of arrays of magnetic dots and exchange bias in nanostructured ferromagnetic-antiferromagnetic structures. Work supported by the U.S. Department of Energy, the National Science Foundation and the Air Force Office of Scientific Research.

4:00 PM N9.7
METAL-INSULATOR TRANSITION IN LaSrMnO THIN FILMS INDUCED BY EPITAXIAL STRAIN AND THE FORMATION OF LSMO QUANTUM DOTS. Hanns-Ulrich Habermeier, Georg, Cristiani, Gudrun Gross, MPI-FKF, Stuttgart, GERMANY.

Pseudomorphically grown perovskite-type thin films can exhibit appreciable interfacial biaxial strain either compressive or tensile, depending on the lattice mismatch of substrate and film, respectively. Tensile stress causes the shift of the Curie temperature to lower values and an increase of the resistivity in LaCaMnO thin films in addition to modifications of the magnetisation curve especially in the range of the Rayleigh law and the approach to saturation. In this contribution, the results of structural, transport and magnetic properties of films under tensile stress of LaCaMnO films are discussed from the point of view of epitaxial stress. Additionally, recent results will be presented showing a film thickness dependent transition from an insulating to a ferromagnetic metallic state in La-Sr-Mn-O thin films of different compositions. The films have been prepared by PLD and analysed by XRD, TEM, transport and Ramanscattering investigations. A generalised picture of the strain generation and relaxation emerges and will be discussed. Using the concepts of epitaxial strain LSMO films of thicknesses below 10 nm have been grown and the formation of LSMO quantum dots with dimensions 3 nm diameter and4nm height have been detected. It could be shown that these quantum dots are ferromagnetic with a Cuiretemperatur well above roomtemperature.

4:15 PM N9.8
STRAIN ACCOMODATION AND RELAXATION MECHANISMS

IN EPITAXIALLY GROWN MANGANITES. Marie-Jose Casanove, Pierre Baules, Christian Roucau, Jerome Majimel, Jean-Claude Ousset, CEMES, CNRS, Toulouse, FRANCE; David Magnoux, Jean-Francois Bobo, LPMC, Toulouse, FRANCE; Manuel Bibes, Josep Fontcuberta, ICMB, Barcelona, SPAIN.

Research on perovskite manganites with general formula $A_{1-x}B_xMnO_3$, where A is a trivalent lanthanide (La, Nd ..) and B a divalent alkaline earth (Sr, Ba, Ca) cation, has known a renewal of activity owing to the recent discovery of their colossal magnetoresistance. The partial substitution of trivalent cations by divalent ones introduces electron holes and leads to the formation of Mn^{4+} ions. The physical properties of perovskite manganites are governed by the Mn^{3+}/Mn^{4+} ratio, which is largely influenced by the chemical composition and the crystallographic distortions. The Mn-O-Mn bond length and angle are of particular importance and both parameters are likely to be adjusted by epitaxial growth induced strain. In this paper, we report the influence of the deposition conditions on the microstructure and state of strain in $La_{0.66}$(Sr or Ca)$_{0.33}MnO_3$ (LSMO or LCMO) layers epitaxially grown on different substrates using RF magnetron sputtering. Particular attention is paid to the influence of deposited thickness, growth rate, annealing under flowing oxygen and nature of the substrate. The magnetic behavior of the films was analyzed before the structural investigation by x-ray diffraction and transmission electron microscopy in its conventional (TEM) and high resolution (HRTEM) modes, performed on plan-view and cross-sectional specimens. It is shown that the epitaxial growth was successfully achieved on the different substrates. As expected, the value of the misfit plays an important part in the state of strain. For instance, fully relaxed layers were always obtained on MgO. On other substrates, misfit relaxation was obtained in samples ex-situ annealed at high temperature. The mechanisms of misfit strain relief strongly vary with the depostion conditions. Above all, structural distortion relaxation due to the rhombohedral or orthorhombic structure of the manganites is observed. Its role in the strain relaxation of the epitaxial layers is discussed.

4:30 PM N9.9
DEVELOPMENT OF ACCELERATED QUANTUM CHEMICAL MOLECULAR DYNAMICS PROGRAM AND ITS APPLICATION TO EPITAXIAL CRYSTAL GROWTH PROCESSES. Momoji Kubo, Hitoshi Kurokawa, Ken Suzuki, Seiichi Takami, Akira Miyamoto, Tohoku Univ., Dept. of Materials Chemistry, Sendai, JAPAN; Akira Imamura, Hiroshima Kokusai Gakuin Univ., Dept. of Mathematics, Hiroshima, JAPAN.

Novel technology on the artificial construction of atomically defined metal oxide layers has been desired in relation to electronic, magnetic, and optical devices. Hence, the atomistic understanding of the epitaxial growth processes of metal oxide surfaces is desired to fabricate atomically controlled structure that exhibits unexplored and interesting physical properties. Previously, we developed an atomistic crystal growth molecular dynamics simulator MOMODY and successfully applied it to the homoepitaxial growth processes of MgO(001), $SrTiO_3$(001), and ZnO(0001) surfaces[1,2]. Moreover, the heteroepitaxial growth system, such as SrO/$SrTiO_3$(001), BaO/$SrTiO_3$(001), MgO/sapphire(0001), Au/MgO(001), etc. are also successfully simulated [3,4]. However, the above classical molecular dynamics approach could not reproduce the surface chemical reactions and electron transfer during the epitaxial growth processes since the empirical interatomic potential is used. Hence, in the present study we developed a new atomistic crystal growth simulator Colors based on our accelerated quantum chemical molecular dynamics methodology. To the best of our knowledge, this is a first simulator to clarify the surface reaction dynamics, low-dimensional structure fabrication, and electron transfer during the epitaxial growth processes. Moreover, we applied it to various heteroepitaxial growth processes on metal oxide surfaces and some new findings which can not be elucidated by experiments were obtained. [1] M. Kubo, Y. Oumi, H. Takaba, A. Chatterjee, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and H. Koinuma, Phys. Rev. B, 61 (2000) 16187. [2] M. Kubo, Y. Oumi, R. Miura, A. Stirling, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and H. Koinuma, J. Chem. Phys., 109 (1998) 8601. [3] M. Kubo, Y. Oumi, R. Miura, A. Stirling, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and H. Koinuma, J. Chem. Phys., 109 (1998) 9148. [4] M. Kubo, Y. Oumi, R. Miura, A. Stirling, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and H. Koinuma, Phys. Rev. B, 56 (1997) 13535.

4:45 PM N9.10
INTERACTION, STRESS, COALESCENCE AND SHAPE TRANSFORMATION OF Ag DOTS ON H-TERMINATED Si(111) SURFACES. J.M. Zuo, B.Q. Li, and Y.F. Shi, Department of Materials Science and Engineering and Materials Research Laboratory, University of Illinois, Urbana, IL.

Growth of stable nanostructures is key to the utilization of their unusual physical properties. As-grown nanoclusters from non-equilibrium kinetic processes are often highly unstable. To understand the stability of nanoclusters and their interactions, we have carried systematic experiments on the shape, orientation, stress and structure of individual Ag nanoclusters grown on hydrogen-terminated Si surfaces. We found that Ag clusters grow in stages from mostly defect-free pyramids to highly symmetrical mounds with twin-boundaries and stacking faults. The amount of stress of each cluster depends on its orientation and size. The number of clusters increases and decreases with the amount of coverage, coalescence occurs when the number of clusters approaches the jamming limit that is determined by the size of clusters and the exclusion zone surrounding each clusters. The morphology of coalescenced clusters suggests an almost liquid-like mobility of large Ag-clusters and a large reorientation of interacting clusters. The experiments were carried using novel electron microscopy and diffraction techniques. The strain of individual nanoclusters was measured by the Moire-fringe techniques. Quantitative electron diffraction, combined with Moire-fringes, was used to determine the orientations of individual clusters, AFM and kinematical electron imaging was used to determine the shapes of clusters. Details of experiment will be presented.