

SYMPOSIUM K

Morphological and Compositional Evolution of Heteroepitaxial Semiconductor Thin Films

April 24 – 27, 2000

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* Invited paper

SESSION K1: SURFACE DYNAMICS-
ATOMISTIC PROCESSES

Chair: M. Dobrowolska
Monday Morning, April 24, 2000
Salon 1/2 (Marriott)

8:30 AM *K1.1

ATOMISTIC AND KINETIC ASPECTS OF METASTABLE STRAINED FILM EVOLUTION. Anupam Madhukar, University of Southern California, Departments of Materials Science and Physics, Los Angeles, CA.

A variety of thin films on solid substrates occur in metastable states accessible during growth. In this talk, I shall focus on an atomistic and kinetic framework for examining the mechanisms of strained film growth. This framework derives heavily from experimental examinations of the InGaAs on GaAs (001) system but should be of value to the general subject of strained semiconductor thin film growth.

9:00 AM *K1.2

DIRECT OBSERVATION OF SUB-CRITICAL FLUCTUATIONS DURING QUANTUM DOT FORMATION. D.E. Jesson, Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN; M. Kaestner, B. Voigtlaender, Institut für Grenzflächenforschung und Vakuumphysik, Forschungszentrum Juelich, GERMANY.

The strain induced roughening of lattice mismatched films during heteroepitaxy is receiving considerable attention as a potential means of fabricating quantum dot arrays for novel device applications. We have directly imaged sub-critical fluctuations which occur during the important nucleation phase of 3D Ge islands grown on Si(001) using scanning tunneling microscopy. Surprisingly, the fluctuations consist of several hundred atoms, even at relatively low growth temperatures, and are consistent with classical nucleation concepts. A new theoretical treatment will be used to describe the subsequent growth and coarsening of quantum dot arrays in the presence of elastic interactions. This has important implications for creating dots of uniform size and spacing.

9:30 AM *K1.3

AB-INITIO STUDIES OF ATOMISTIC PROCESSES IN III-V EPITAXIAL GROWTH. N.A. Modine, Sandia National Laboratories, Albuquerque, NM; Hanchul Kim, E. Kaxiras, Harvard Univ., Cambridge, MA.

We review recent progress in using density functional theory (DFT) based electronic structure methods to identify and characterize the atomistic processes that control epitaxial growth of III-V semiconductors. We focus on MBE growth of AlSb at the (001) surface as a representative system. Surface reconstructions, adatom behaviors, and island nucleation mechanisms are addressed. We compare the relatively well studied group-III arsenides to our results for antimonides and show that these superficially similar systems have surprisingly different behaviors. Our DFT results support and help to clarify recent atomic-resolution STM results obtained at the Naval Research Laboratory. Of particular interest to researchers in heteroepitaxy, we show that effects of varying the Fermi energy and strain can be included straightforwardly when calculating the relative stabilities of competing structures. We also briefly report on efforts within DARPA's Virtual Integrated Prototyping initiative to use Kinetic Monte-Carlo and Level Set methods to bridge to longer length scales. Finally, we consider some remaining challenges in ab-initio investigations of epitaxial growth and mention some promising approaches to overcoming these difficulties. 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.

10:15 AM *K1.4

HIGHLY ORDERED UNIFORM QUANTUM DOTS INDUCED BY ION SPUTTERING. H. Kurz, S. Facsko, T. Dekorsy, Institute of Semiconductor Electronics, RWTH Aachen, Aachen, GERMANY.

Ion sputtering of surfaces produces various morphologies within which regular ripple structures have attracted much interest in recent years. Ripple formation has been observed for non-normal incident ion bombardment in a wide variety of materials. We investigated the morphology of GaSb surfaces during low energy ion sputtering at normal incidence and observed the formation of highly ordered dot patterns [1]. The diameters of these dots have a narrow distribution and range from 10 nm to 100 nm depending on the process parameters. The primary stage of the pattern evolution are small dots already hexagonally ordered which grow in diameter until a stable closely packed pattern is reached. The experimental observations are explained by the noisy Kuramoto-Sivashinsky equation which successfully predicted the periodic ripple structures and kinetic

roughening [2]. The dependence of the wavelength on ion-energy predicted by this equation is confirmed by our experiments. This is a clear evidence for the relevance of the higher order ($n=4$) derivative of the surface contour for the regular dot formation. The narrow size distribution and the crystallinity of the dots make the presented method attractive for the fabrication of quantum dots by direct patterning of semiconductors.

[1] S. Facsko, T. Dekorsy, C. Koerdt, C. Trappe, H. Kurz, A. Vogt and H.L. Hartnagel, Science 285, 1151 (1999).

[2] M.A. Makeev and A.-L. Barabasi, Appl. Phys. Lett 71, 2800 (1997).

10:45 AM *K1.5

QUANTUM DOT AND HOLE FOR DOT AND HOLE FORMATION IN SPUTTER EROSION. B. Kahng, Department of Physics and Center for Advanced Materials and Devices, Konkuk University, Seoul, KOREA.

Recently it was experimentally demonstrated that sputtering under normal incidence leads to the formation of spatially ordered uniform nanoscale islands or holes. Here we show that these nanostructures have inherently nonlinear origin, first appearing when the nonlinear terms start to dominate the surface dynamics. Depending on the sign of the nonlinear terms, determined by the shape of the collision cascade, the surface can develop regular islands or holes with identical dynamical features, and while the size of these nanostructures is independent of flux and temperature, it can be modified by turning the ion energy.

11:15 AM K1.6

PRE-DOTS: KINETIC PATHWAY BETWEEN WETTING LAYER AND COHERENT Ge ISLAND GROWTH ON Si(001). A. Vailionis, B. Cho, G. Glass, P. Desjardins, David G. Cahill and J.E. Greene, University of Illinois, Department of Materials Science and the Materials Research Laboratory, Urbana, IL.

We use in-situ scanning tunneling microscopy (STM) and Rutherford backscattering spectroscopy (RBS) to characterize the initial stages of Ge deposition on Si(001) by gas-source molecular beam epitaxy. In much of the experimental and theoretical literature, the transition from the two-dimensional pseudomorphic wetting layer to three-dimensional coherent islands has been assumed to take place by abrupt nucleation of pyramidal-shaped Ge islands bounded by {105} facets; subsequent shape transitions from pyramids to larger and more hemispherical dome shapes have also been studied extensively. Our experimental results indicate that the appearance of pyramids is not abrupt but takes place through a three-dimensional islands with a height-to-width ratio that is approximately one-half that of pyramids. We observe pre-dots only for an extremely narrow range of film coverage, 3.7-3.9 monolayers (as measured by RBS); at slightly higher coverages, pyramids dominate the surface morphology with an areal density comparable to the areal density of pre-dots while at lower coverages the Ge wetting layer is flat and exhibits an MxN reconstruction. The average diameter of the pre-dots is 18 nm; when scaled by the strain energy, this size is comparable to the length scales observed by Floro and co-workers in the initial roughening of $\text{Si}_{1-x}\text{Ge}_x$ alloys on Si(001).

11:30 AM K1.7

AN AB-INITIO APPROACH FOR ELASTIC INTERACTION BETWEEN DEPOSITED ATOMS ON A SILICON <100> SURFACE. Laurence Magaud, LEPES CNRS, Grenoble, FRANCE; Alain Pasturel, CNRS, Université Joseph Fourier, Grenoble, FRANCE; Philippe Peyla, McGill Univ., Montreal, CANADA; Chaouqi Misbah, Laboratoire de Spectrométrie Physique, CNRS, Université Joseph Fourier, Grenoble, FRANCE.

Elastic interactions between atoms deposited on a thin Silicon <100> layer is investigated. As it was previously predicted by Peyla et al [Phys. Rev. Lett. 82, 787 (1999)] by continuum elasticity theory, defects deposited on thin layers may either attract or repel each other. This interaction depends both on the layer thickness and on the local geometric force distribution around the deposited atom (considered as a defect because it distorts the layer underneath). Each atom i of the layer is free to relax, i.e. with a displacement vector u_i . If $u_i \ll a$ (a being the lattice parameter) the relaxation is considered as elastic, resulting in an interaction between the defects. More complicated relaxation can also occur with $u_i > a$, resulting in surface reconstructions. The latter phenomenon is a highly non-linear effect which can affect the elastic constants of the surface. Ab-initio approach allows to describe properly this problem which depends strongly on the specificity of the investigated material. Here, we propose to apply such an approach on a Si-layer, standing coherently on a hard substrate, on which we deposit Si or Ge atoms.

11:45 AM K1.8

ISLAND-ADATOM ELASTIC INTERACTION EFFECTS IN

THIN-FILM GROWTH. Alonso D. Peralta, State University of New York, Dept. of Mechanical Engineering, Stony Brook, NY.

One of the most fundamental processes in thin film growth is the migration of the deposited adatoms on a substrate. A clear understanding of the mechanisms influencing this process is essential for the growth of atomically flat layers needed in semiconductor applications. We have investigated the role elastic interactions among surface defects play in this process. Surface defects corresponding to adatoms, vacancies and steps interact elastically, affecting and often dominating the kinetic processes associated with thin-film growth. Result for the island-adatom elastic interactions are presented for the adatoms on top of the island, and on the terraces in the immediate vicinity of the island as well as in the far field. For homoepitaxial islands that are formed by a pair of opposite steps, the elastic interaction energy suggest conditions for which interlayer transport is favored for small islands; similar results are found for heteroepitaxial islands in tension. For heteroepitaxial islands in compression, the edge barrier for interlayer transport exhibits a maximum for intermediate length scales. In the case of flat homoepitaxial islands of circular shape adatom diffusion towards the edge of the island is favored along the (110) orientation, driving the adatoms towards the more jagged edge of the island. Implications of these interactions for thin film growth are discussed.

SESSION K2: GROWTH ON PATTERNED, HIGH INDEX, AND VICINAL SUBSTRATES

Chair: Anupam Madhukar
Monday Afternoon, April 24, 2000
Salon 1/2 (Marriott)

1:30 PM *K2.1

STRAIN ENGINEERING IN HETEROEPITAXIAL GROWTH OF GeSi ON Si(001) USING TEMPLATES, COMPLIANT SUBSTRATES, AND SILICON-ON-INSULATOR. Max G. Lagally, University of Wisconsin-Madison, Madison, WI.

The use of strained semiconductor thin films promises significant advantages in fast electronic devices. We are investigating the underlying atomistic mechanisms in "strain engineering" thin films of SiGe and Ge on Si(001) grown by both CVD and MBE in order to optimize electronic and optoelectronic properties. To assess other possible stress control parameters, we have begun to grow films on silicon-on insulator (SOI) substrates and on lithographically patterned regions of Si(001). Using force and tunneling microscopies, low-energy electron microscopy, and electron and x-ray diffraction, we characterize surface strain fields and surface/interface structures and morphologies, as well as the influence of patterning and use of SOI, on nucleation and growth of both 2D and 3D morphologies. Using simple device structures made from these films, we have begun to correlate electronic and optoelectronic properties with morphology and strain. Finally, we discuss theoretical analyses and simulations based on elastic models to elucidate formation and self-organization processes driven by strain relaxation.

Supported by NSF, ONR, and AFOSR

2:00 PM K2.2

NOVEL APPROACH TO NANOMETER-SCALE PATTERNING OF SILICON SUBSTRATES. Andrey S. Bakin, Dirk Piester, Ingo Behrens, Hergo-Heinrich Wehmann, Detlef Fehly, Erwin Peiner and Andreas Schlachetzki, Institute for Semiconductor Technology, Technical University of Braunschweig, Braunschweig, GERMANY; Hans-Joachim Rösler, Institute of Material Science, Technical University of Braunschweig, Braunschweig, GERMANY.

The heterostructures of direct band-gap material as InP on indirect band-gap silicon are of great interest for a new generation of optoelectronic devices monolithically integrated with silicon microelectronics. Severe obstacles arise from the large mismatch in lattice parameter and thermal expansion coefficient between layer and Si substrate which lead to the formation of lattice defects and residual stress. Different approaches were employed to grow high quality InP on Si. One of them is the growth on a patterned substrate. Initially we have investigated and developed selective maskless etching of (001) Si substrates in a NaOH based etchant in order to obtain micrometer-scale pyramids faceted by (111)-planes. InP layers have been grown on such patterned Si substrates using metal-organic vapor phase epitaxy (MOVPE). The samples were investigated using atomic-force microscopy (AFM), scanning electron microscopy, transmission electron microscopy, and defect etching. Further improvements of the InP layer quality are possible if smaller size patterning and also pyramids faceted by other than (111)-planes could be employed. We developed a new approach to the nanometer-scale patterning of the Si substrates and results of this study are discussed in the present paper. We used self-assembled nanometer-scale

three-dimensional InP islands as a mask for further Si substrate patterning. InP islands were grown by MOVPE at 400 °C and then transformed during annealing at 640 °C. The samples were etched under different temperatures and durations in two etchants: KOH- and NaOH-based. AFM was used to determine the morphology of the samples and to evaluate the dimensions of the etched pyramids. The results obtained are discussed. It is shown that three-dimensional InP islands grown on Si substrate by MOVPE provide an excellent self-assembled mask for further nanoscale patterning of the silicon substrate.

2:15 PM K2.3

STRAIN INDUCED COMPOSITIONAL MODULATIONS IN AlGaAs OVERLAYERS INDUCED BY LATERAL SURFACE GRATINGS. Ute Zeimer, Lars Hofmann, Ferdinand-Braun Institut für Höchstfrequenztechnik, Berlin, GERMANY; Ullrich Pietsch, Jörg Grenzer, Institut für Physik, Universität Potsdam, Potsdam, GERMANY.

The strain and compositional modification of $Al_xGa_{1-x}As$ layers have been studied after the overgrowth onto a laterally patterned GaAs[001] substrate. The surface-wire structure of GaAs was defined along the [-110] direction via a photolithographic process and subsequent wet-chemical etching. An additional heat treatment at 670 °C (MOVPE growth temperature) results in a sinusoidally shaped grating with a period of about 200 nm and a modulation depth of about 60 nm. The patterned substrate was overgrown with $Al_xGa_{1-x}As$ in an MOVPE reactor in horizontal geometry using trimethylgallium, trimethylaluminum and arsine as precursors and hydrogen as carrier gas. The chosen growth time corresponds to a layer thickness of about 125 nm. After the overgrowth process the sample surface appears smooth without a periodic undulation. Nondestructive sample inspection was performed by high-resolution X-ray grazing-incidence diffraction at the BW2 beamline at HASYLAB (Germany) recording two symmetry-equivalent in-plane Bragg reflections. Whereas the transversal scan (ω -scan) across the (220) Bragg peak provides the lateral density modulation the respective longitudinal scan ($\omega/2\theta$ -scan) across the (-220) peak measures the lateral strain profile in addition. Both can be obtained as a function of depth below the surface [1]. The longitudinal scans show distinct grating side peaks. They are originated from the appearance of a periodic strain field within the overlayer induced by the buried GaAs grating. The grating peaks in the transversal scans can only be explained by the existence of a periodic compositional modulation [2]. Besides different growth velocities at differently indexed crystallographic planes [3] a strain-dependent segregation coefficient of aluminium may be one of the origins of our finding. In this talk we present systematic investigations of this behavior for samples with different aluminium content.

[1] N. Darowski, K. Paschke, U. Pietsch, K.-H. Wang, A. Forchel, D. Lübbert and T. Baumbach, *Physica B* 248, 104 (1998)

[2] N. Darowski, U. Pietsch, U. Zeimer, V. Smirnitzi and F. Bugge, *J. Appl. Phys.* 84, 1366 (1998)

[3] L. Hofmann, A. Knauer, I. Rechenberg and M. Weyers, *J. Cryst. Growth* 195, 485 (1998)

2:30 PM K2.4

ATOMIC FORCE MICROSCOPY CHARACTERIZATION OF INTERFACE ROUGHNESS OF V-SHAPED AlGaAs/GaAs QUANTUM WIRE. Xue-Lun Wang, Mutsuo Ogura, Tsukuba, JAPAN.

The interface quality of semiconductor heterostructures influences severely their optical and electronic properties, which is especially critical for quantum wires (QWRs) and quantum dots (QDs) due to the increased number of heterointerfaces. In this work, we investigated the effects of $NH_4OH:H_2O_2:H_2O$ (=1:3:50) etching of the initial V-grooved substrate and the use of an AlGaAs/GaAs short-period superlattice buffer layer on the improvement of interface uniformity of V-shaped AlGaAs/GaAs QWRs by direct atomic force microscopy (AFM) observation of the QWR surface. We first investigated the surface morphology of the initial V-grooved substrate before growth and found that the surface roughness on the initial V-grooved substrates induced during V-groove preparation processes can be reduced greatly by the use of NH_4OH etching treatment. Next, thick GaAs QWRs (80nm) were grown by flow rate modulation epitaxy and their surface morphologies were investigated again by AFM observation. It was found that the width of the (001) QWR facet can be widened by a factor of 2 and the monolayer step islands formed on the (001) QWR facet can be elongated by a factor of as large as 10 by the use of the NH_4OH etching treatment. It was also found that the formation of large quasi-periodic step arrays on the (311)A QWR facets resulted from step bunching effects can be effectively suppressed by the combined uses of the NH_4OH etching treatment and an AlGaAs/GaAs short-period superlattice buffer layer. The above improvements of QWR interface quality were also confirmed by micro-photoluminescence measurements.

3:15 PM *K2.5

LAYER-BY-LAYER GROWTH AND PATTERN PROPAGATION. Dietrich E. Wolf, Gm-Universitat Duisburg, Duisburg, GERMANY.

Recent Monte Carlo results on layer-by-layer growth and the propagation of surface patterns in molecular beam epitaxy as well as in pulsed laser deposition will be presented. They indicate that previously suggested scaling exponents for the damping time of RHEED-oscillations and for the optimal pattern scale fail, and the theory needs to be modified.

3:45 PM K2.6

ISLAND COALESCENCE INDUCED SUBSTRUCTURE WITHIN GaP EPITAXIAL LAYERS GROWN ON (001), (111), (110) AND (113) Si. V. Narayanan¹, S. Mahajan¹, K.J. Bachmann², V. Woods³, N. Dietz³. ¹Department of Chemical, Bio and Materials Engineering, Arizona State University, Tempe, AZ; ²Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC; ³Department of Physics, North Carolina State University, Raleigh, NC.

GaP islands grown on selected surfaces of Si and their coalescence behavior have been investigated by transmission electron microscopy. These layers were grown by chemical beam epitaxy. A number of significant observations emerge from this study. First, planar defect formation has been shown to be related to stacking errors on the smaller P-terminated {111} facets of GaP islands. Amongst the four orientations, (111) epilayers have a higher density of stacking faults and first order twins because of more P terminated {111} facets per island. Second, twinning on exposed {111} facets can produce multiply twinned regions when islands coalesce. Third, symmetric twin boundaries identified as second and third order twins are seen within (111) and (110) layers. Formation of such defects is attributed to successive twinning on differently inclined {111} planes. Fourth, inversion domain boundaries lying on {110} planes have been shown to form during GaP island coalescence across monatomic steps on (001) Si. Image simulations have been performed to show that these boundaries can be seen in high resolution lattice images and the observed contrast is attributed to the presence of wrong Ga-Ga and P-P bonds at the inversion boundary. The authors gratefully acknowledge the support of this work by DOD-MURI grant F49620-95-1-0447.

4:00 PM K2.7

SELF-ORGANIZED STRIP-LIKE InAs NANOSTRUCTURES GROWN ON InP VICINAL SURFACES BY MOVPE. Laurent Auvray, Veronique Soulière, Hervé Dumont, Jacques Dazord, Yves Monteil, Jean Bouix, LMI UCB Lyon1, Villeurbanne Cedex, FRANCE.

We have investigated the influence of MOVPE growth parameters on the surface morphology of InAs nanostructures grown on 0.2° misoriented (001)InP substrates. The experiments were performed in a horizontal LP-MOVPE reactor using a 80% N₂/20% H₂ mixture as carrier gas. Thin layers of InAs (nominal thickness of about 3 and 6 ML) were deposited at 500° C with V/III flux ratios ranged from 25 to 125. The sample was cooled down from 500 to 350° C during 6 minutes under either arsine or phosphine atmosphere. The influence of this step has been found to greatly determine the surface morphology of the nanostructures observed by AFM. All 3 ML thick InAs deposit cooled down in arsine atmosphere exhibits a step-bunched terrace-like morphology with regular step front. Dots of large diameter (610 nm) and height (50 nm) are obtained with a low density (4x10⁷ cm⁻²). In contrast, when the same layer is cooled down from the growth temperature to 350° C in a phosphine flux, no dots are observed. The surface exhibits a bunched terrace-like morphology with a quite irregular step front. When increasing the nominal layer thickness (to about 6 ML), dots of 129 nm diameter and 10 nm height are observed with a density of 3x10⁸ cm⁻². They appear to be self-aligned along the steps, forming a non continuous stripe, regularly spaced every 3-4 terraces. The wetting layer step front is always quite irregular. The morphology of the stripe obtained can be varied with the growth conditions (V/III flux ratio). In this work, we will propose a mechanism for the formation of the stripe observed during the cooling under phosphine atmosphere.

4:15 PM K2.8

A MICROMECHANICAL MODEL OF SURFACE STEPS UNDER THE INFLUENCE OF STRESS. R.V. Kukta, State University of New York, Mechanical Engineering, Stony Brook, NY; K. Bhattacharya, California Inst of Technology, Div of Engineering and Applied Sciences, Pasadena, CA.

An elastic theory of steps on a crystal surface is presented which provides new insight to the complex three-dimensional morphologies which develop during thin film growth. A step is viewed as a line

source of stress which is constrained to move on the surface of an elastic half-space. The theory is formulated with careful consideration for the long ranged elastic field produced by a step and for the energetic force driving step motion. The elastic field produced by a step consists of its self-stress, which is independent of all other fields, and the elastic response of the step to all sources stress, including itself. The paper focuses on morphological evolution during crystal growth as governed by the energetic force on a step as it interacts with a uniform mismatch, with other steps, and with itself. Through analytical calculations and numerical simulations, it is shown that the model predicts many experimentally observed microstructural features such as complex step bunching patterns, deep grooves between merging islands, and the stress induced waviness of a step train.

4:30 PM K2.9

STRAIN ENGINEERING SiGe 3D ISLANDS USING PATTERNED Si ON INSULATOR (SOI) SUBSTRATES. P. Rugheimer, P. Moran, D.E. Savage, V. Zielasek, A.R. Woll, T.F. Kuech and M.G. Lagally, University of Wisconsin-Madison, Madison, WI; E. Mateeva, Colorado School of Mines, Golden, CO.

Self-organized 3D islands form in order to relieve misfit strain during heteroepitaxial growth of SiGe on Si(001). While kinetic factors such as substrate temperature and deposition rate can influence island size and spatial distribution, misfit strain plays the dominant role in determining final film morphology. In this work, we use patterned SOI substrates to mediate strain and influence film morphology. Films are grown, using both MBE and CVD, on lithographically defined mesas with lateral dimensions ranging from 5 to 200 microns patterned onto both 16nm Si on SiO₂ bonded-wafer substrates and Si(001) control substrates. Film morphology is followed in-situ with RHEED and ex-situ with AFM and CTEM. We find that growing on the patterned SOI wafers increases dramatically the critical thickness for island formation. This influence is much less for growth on the patterned Si(001) control substrate as well as growth on unpatterned SOI. Possible mechanisms such as short-range viscous compliance as well as mediation of dislocations will be discussed. Supported by NSF-MRSEC and by ONR

4:45 PM K2.10

STEP BUNCHING, CHEMICAL ORDERING, AND DIFFUSIVITY IN THE Si_{1-y}C_y/Si HETEROEPITAXY. Frank Grosse, UCLA, Dept of Mathematics, Los Angeles, CA; Edward T. Croke, Mark F. Gyure, HRL Laboratories, Malibu, CA; Margaret Floyd, David J. Smith, Arizona State University, Tempe, AZ.

The epitaxial growth of Si on high index surfaces is studied and theoretically described under presence of low concentrations of C (1% - 10%). Experimentally, step bunching on (118) surfaces is observed. The length of the (001) terraces separating the step bunches are self-adjusting depending on growth temperature, flux rates and C concentration. Furthermore, TEM cross sectional views suggest a chemical ordering, i.e. equidistant (001) planes with high C concentration separated by nearly pure Si layers in the grown structure. The physical origin of the step bunching is explained by an effective increase of the Si diffusivity with local C concentration caused by local strain surrounding the C atoms. Assuming a low C diffusivity, the local C concentration is increased with exposure time of the local facet. Higher C concentration means higher Si diffusivity. Steps surrounded by areas with lower (higher) C concentrations grow faster (slower) and the difference in C concentration increases even more. The C atoms incorporate primarily at the emerging (001) terraces and are buried by the growing step bunches formed by pure Si, resulting in the chemical ordering described above. To check our model we carried out kinetic Monte-Carlo simulations on a fcc lattice with two species. The interaction is described within a simple linear bond counting model. We do not include a Schwoebel barrier. Furthermore step exchange processes and desorption are forbidden; only adsorption (growth) and diffusion are allowed to make the model as simple as possible in order to find the necessary processes to describe chemical ordering connected with step bunching. In comparison with the experiment we found excellent agreement with the variation in the overall C concentration, temperature, flux rates and tilt angle.

SESSION K3: QUANTUM DOTS I

Chair: R. Stanley Williams
Tuesday Morning, April 25, 2000
Salon 1/2 (Marriott)

8:30 AM *K3.1

ALLOY COMPOSITION IN SELF-ASSEMBLED QUANTUM DOTS. J. Tersoff, IBM-T.J. Watson Research Center, Yorktown Heights, NY.

In heteroepitaxy, misfit strain leads to formation of islands. When capped, these can serve as self-assembled quantum dots. However, the composition of the dot may differ considerably from the nominal

composition of the deposited material. Even more importantly, the composition within a quantum dot may be highly non-uniform. In that case, the effective shape and size of the quantum dot (i.e. of the confining potential for electrons and holes) is radically different than the nominal shape and size of the island. This talk will present theoretical results for the composition profile, and its relation to the thermodynamics and kinetics of island growth. The shape of the composition profile within the quantum dot may be understood from simple and rather general arguments. A more detailed calculation confirms these general features, and predicts a composition distribution very similar to that seen in recent experiments. The effect of capping on the composition and shape of the dot will also be discussed.

9:00 AM *K3.2

THE EVOLUTION OF THIN FILMS DURING HETEROEPITAXY: FROM PLANAR FILMS TO DOTS. J.J. Eggleston and P.W. Voorhees, Northwestern Univ, Evanston, IL.

Many semiconductor films evolve by the Stranski-Krastanov process whereby a planar film breaks up into an array of islands. A driving force for this process is the relief of the elastic stress generated by the film-substrate misfit. The morphological evolution of a planar film to one consisting of an array of islands is a highly nonlinear process. As a result, a fully numerical solution of the equations governing surface energy and elastic energy driven surface diffusion is required to follow the island formation process. Moreover, it is clear that in many semiconductors the surface energy is highly anisotropic, giving rise to strongly anisotropic island morphologies. A phase field model for thin film growth has been developed with which the evolution of an elastically stressed film with a highly anisotropic surface energy can be determined. The calculations show the formation and evolution of nearly faceted islands and the crucial role played by anisotropy in the evolution of the film. The implications of these results on quantum dot formation will be given.

9:30 AM K3.3

THE STABILITY OF QUANTUM DOT ARRAY AGAINST COARSENING AND SHAPE TRANSITION. Cheng-hsin Chiu, Institute of Materials Research and Engineering, SINGAPORE.

The nano-structure of self-assembled quantum dots has many potential applications in novel semiconductor devices. A pivotal task in realizing these applications is to control the uniformity of the dot size and the dot shape. The task, however, is challenging since experimental observations seem to indicate that dots tend to coarsen and/or transform into different shapes during the growth and the subsequent annealing process. In order to overcome the difficulties, it is necessary to have an insight into the stability of island arrays against coarsening and shape transition. This issue is examined in this paper by considering both the phase diagram of the equilibrium island arrays and the morphological evolution of the heteroepitaxial islands. In the study of phase diagram, the equilibrium structure is determined by analyzing the free energy, consisting of the strain energy, the surface energy, and the film-substrate interaction energy, of a quantum dot array characterized by the wetting layer thickness, the dot spacing, the dot size, and the dot shape. The results show that there are four types of equilibrium structures. The first one is a hut island array that is stable against coarsening and shape transition; the second one is a stable dome island array. The equilibrium structure can also be a mixture of hut and dome islands stable against coarsening. And the fourth type of structure is coarsening islands. The regimes of material properties corresponding to the four structures constitute the phase diagram of the island morphologies. The implications of the phase diagram on improving the stability of island arrays against coarsening and shape transition are discussed. In the second part of the talk, we employ simulations to show that the four types of structures as mentioned above can occur during the annealing process. The simulations, focused on the morphological evolution of a Stranski-Krastanow system, are based on a continuum approach in which the effects of different energetic forces on the morphological evolution are represented by the surface chemical potential. The simulations demonstrate that the morphological evolution can lead to a steady state of uniform and regular hut (or dome) islands or a mixture of hut and dome islands. We also present simulations for the island coarsening process. In the first case, the islands coarsen but the shape remains as a hut, while in the second one, the hut-dome transition occurs.

9:45 AM K3.4

MONTE CARLO SIMULATION OF HETEROEPITAXIAL GROWTH OF SEMICONDUCTOR COMPOUNDS WITH LARGE MISMATCH. Rachid Malek, Physics and Astronomy Department, Clipping Labs, Ohio University, Athens, OH; M. Djafari-Rouhani, Daniel Estève, Laboratoire d'Analyse et d'Architecture des Systèmes LAAS, Toulouse, FRANCE.

We have performed atomic scale simulation of the heteroepitaxial growth of semiconductor systems with large mismatch by associating Monte Carlo, MC, method with an energetic model derived from the Valence Force Field, VFF, approximation. The energy model allows us to determine stress and strain in the deposited film by minimizing the total energy, and to calculate the stress dependent probabilities. The MC technique is needed to describe the kinetic of growth, and thus to handle the random nature of the atomic motions based on Arrhenius law and Poisson process. We have shown that the growing film presents 3D islands or cavities with (111) facets. In the first case, the interlayer migrations avoid coalescence of clusters to form a planar film and favor the formation of large and high islands. In the second case, the cavities are filled by the growth of (111) facets and lead to the formation of point defects, like a bulk vacancies, and their association to form extended defects, like a vacancy lines and vacancy clusters. The creation of these defects is related to atoms in hanging positions which are the results of reactions between atoms in interstitial positions. The strain relaxation is shown to be performed in few atomic layers and not uniform inside a given island. The maximum strain relaxation is located in the border of these islands where the strain energies are small and the atomic displacements are large.

10:30 AM *K3.5

NEW TOOLS TO CONTROL MORPHOLOGY OF SELF-ORGANIZED QUANTUM DOT NANOSTRUCTURES. Dieter Bimberg, Vitaliy Shchukin, Technische Universität Berlin, Berlin, GERMANY.

New growth methods are introduced which include the growth of multi-layered arrays of 2D islands, the seeding of quantum dots (QDs), activated phase separation of alloys, etc. These methods allow efficient wavefunction engineering of localized excitons in QDs and are of high practical importance for fabrication of QDs for optoelectronic applications. (I.) We have grown and studied ultra-thin insertions comprised of 2D (1-3 monolayers high and nanometer-scale wide) islands embedded in a wide bandgap matrix. Complex studies by high resolution electron microscopy (HREM) followed by DALI processing, theoretical modeling of growth, photoluminescence (PL) and calorimetric reflection (CR) spectroscopy unambiguously confirm [1] that multi-layered arrays of CdSe:ZnSe islands and InAs:GaAs islands exhibit transitions from vertical correlation to vertical anticorrelation driven by variation of the spacer thickness. (II.) Drastically different temperature dependence of the size and the density of QDs for equilibrium arrays of islands and for kinetic-controlled arrays allows to distinguish the two mechanisms of formation. HREM measurements, theoretical modelling, and PL spectroscopy of arrays of 2D InAs:GaAs islands confirm the equilibrium nature of these arrays. (III.) For 3D islands obtained in the Stranski-Krastanow growth mode, correlated growth allows to use the concept of seeding of the QDs [2]. E. g., the growth of the first several sheets of InAlAs on GaAs(001) leads to a dense array (10^{12} cm^{-2}) of very small islands which serve as stressors for the growth of InGaAs islands in the subsequent sheets. Seeding creates an additional possibility to control separately the size and the density of islands and to obtain an array of conventional InGaAs QDs of ultrahigh density. (IV.) The overgrowth of InAs/GaAs(001) QDs by GaAlInAs alloy results in a substantial redshift of the PL peak despite the increase in the bandgap of the surrounding matrix. Cross-sectional TEM studies have confirmed i) an effective increase in the lateral size of QDs and ii) formation of In-rich domains on top of QDs. Both effects are due to the phase separation of GaAlInAs activated by InAs stressors. The application of these newly discovered tools presents the potential of practical control and tuning of geometrical parameters and electronic spectra of the QDs and enables us to fabricate QD lasers which surpass now conventional quantum well lasers. [1] V.A. Shchukin and D. Bimberg. Rev. Mod. Phys. 71, 1125 (1999). [2] M.V. Maximov et al. Proc. 24th Int. Conf. on Physics of Semiconductors, August 2-7, 1998, Jerusalem, Israel. Ed. D. Gershoni, World Scientific, Singapore, CD-ROM, Section VII: One- and Zero-dimensional Systems; Subsection B: Optical Studies of Wires and Dots, No. 34.

11:00 AM K3.6

MORPHOLOGICAL EVOLUTION OF HIGHLY STRAINED InSb/InAs (001). Aruna Seshadri, Joanna Mirecki-Milunchick, University of Michigan, Department of Materials Science and Engineering, Ann Arbor, MI.

We investigated the morphological evolution of InSb grown on InAs (001) substrates (lattice mismatch = 6.9%) as a function of film thickness. All films were grown at approximately 400°C using solid source MBE, at a growth rate of 0.4 ML/sec and antimony to indium ratio on the order of 2.5 to 1. Due to the very large lattice mismatch, growth proceeded via the Volmer-Weber mode. At the lowest thicknesses, large rectangular islands with flat tops were observed. For instance, the 5 nm film had islands nominally 300 nm long, 120 nm wide and 36 nm tall. At 10 nm, the islands evolved into long mesas aligned parallel to the [110], with a nominal width of 200 nm, average

height of 75 nm and length on the order of microns. For both these films the size and density of the features are disproportionately large compared to the volume of material deposited, indicating that the InAs buffer layer interacts with the InSb film. As the thickness of the films increased these features coarsened. At a thickness of 100 nm, the morphology transformed into spiral, pyramidal structures that are approximately 1200 nm x 800 nm at the base and 2-4 nm tall. The reduced height indicates that the features have coalesced. The spiral nature of the pyramids implies the presence of screw dislocations penetrating through the film. These data demonstrate that the morphological evolution of the film is significantly different from other films with similar lattice mismatch, such as InAs/GaAs. We propose that this difference is due to lower surface energy and higher diffusivity of InSb.

11:15 AM **K3.7**

MORPHOLOGICAL STABILITY OF 3D InAs ISLANDS GROWN ON GaAs. J.B. Smathers, H. Yang, C. Workman, G.J. Salamo, Department of Physics, University of Arkansas, Fayetteville, AR.

Fundamental issues regarding self assembled 3D islands that result from strained epilayer growth remain unresolved. Recently the detailed nanocrystalline structures of Ge and InAs islands, on Si and GaAs substrates respectively, have been resolved. In this work we address the issue of the stability of such InAs nanocrystals which form on GaAs(001). Some reports claim the islands continually ripen owing the strain reduction scaling more rapidly than the island surface energy cost as a function of increasing island volume. Alternatively, others have claimed that under certain conditions the surface morphology can be stabilized, so that the islands become laterally ordered and ripening is suppressed. Using a combined molecular beam epitaxy and scanning tunneling microscopy facility we have systematically investigated the nature of island ripening as a function of both As pressure and substrate temperature to clarify this issue.

11:30 AM **K3.8**

SHAPE TRANSITION OF InAs ISLANDS ON InP (111)A. Hanxuan Li, Theda Daniels-Race, Department of Electrical & Computer Engineering, Duke University, Durham, NC; Mohamed-Ali Hasan, Department of Electrical & Computer Engineering & The Cameron Applied Research Center, The University of North Carolina, Charlotte, NC.

Recent progress in strained island formation has led to new theoretical and experimental advances, as well as to promising materials for various optoelectronic applications. The (111) orientation is of particular interest. In this work, the self-organization of InAs/InP (111)A system is investigated. The samples were grown by a MBE system on InP (111) substrates. After the growth of a lattice-matched AlInAs buffer layer, 2-6 monolayers of InAs were grown. Atomic force microscopy (AFM) and transmission electronic microscopy (TEM) reveal that InAs islands, as they grow in size, undergo a shape transition. Below a critical size of ~ 30 nm, round-shaped quantum dots form, while above this size they grow in the shape of equilateral triangles, reflecting the symmetry of the (111) substrates. The edges of the triangular islands are aligned along the three equivalent $\{110\}$ directions of the (111) surfaces. The shape transition is discussed in terms of surface and interfacial energies, and ascribed to the island size dependence of strain relaxation. This work is partially supported by NSF grant #NSF-ECS-96-33780 and the Department of Energy grant #DE-FG02-97ER45648.

11:45 AM **K3.9**

CARBON-INDUCED Ge ISLANDS ON Si(001) GROWN BY LPCVD. Michael Goryll, Lili Vescan, Hans Lueth, Research Centre Juelich, Institute of Thin Films and Ion Technology, Juelich, GERMANY.

Self-organized island growth is of particular interest, as nanometer-scale structures can be produced during epitaxy. To remain compatible with the existing Si technology, the SiGe system is favorable. Up to now, the problem using Ge islands on Si was that the island size could not be reduced easily. To observe quantum size effects the islands have to be very small (typical dimensions of approx. 10-20nm). The use of a sub-monolayer of carbon deposited prior to Ge growth in MBE has shown promising results: the island size was reduced significantly while the areal density was increased. Our goal was to investigate the role of a carbon layer on Ge island growth on Si(001) using low pressure chemical vapor deposition (LPCVD). Propane (C_3H_8) diluted in He was used as a carbon source. Calibration measurements of carbon incorporation into a SiGeC layer were performed at 700°C. Measurements of the degree of elastic relaxation of these layers by X-ray scattering and by photoluminescence will be presented. For the island growth studies, the Si surface was carbonized at 700°C. The growth temperature of the subsequent Ge layer varied in the range between 600°C and 700°C. AFM investigations showed that the influence of the carbon

layer was most significant at low growth temperature. Small-sized islands with a narrow size distribution could be achieved using a carbon layer. Compared to a sample grown without this layer, the size distribution was significantly broader. An enhancement of the growth rate of the Ge layer, as seen from Rutherford backscattering analyses (RBS) will be discussed.

SESSION K4: QUANTUM DOTS II

Chairs: Jerry Tersoff and Albert-Laszlo Barabasi
Tuesday Afternoon, April 25, 2000
Salon 1/2 (Marriott)

1:30 PM ***K4.1**

QUANTUM DOT FORMATION IN THE InAs-GaAs SYSTEM - STRAIN IS NOT THE ONLY FACTOR. Bruce Joyce, Dimitri Vvedensky, Dept of Physics, Imperial College, London, UNITED KINGDOM; Gavin Bell, Pippa Steans, Dept of Chemistry and Centre for Electronic Materials and Devices, Imperial College, London, UNITED KINGDOM.

The commonly accepted mechanism of coherent quantum dot formation is via a Stranski-Krastanov process of strain relaxation. This does not, however, explain why in the InAs-GaAs system QDs only form on As-stable reconstructions of (001) oriented surfaces. On all other low index surfaces strain relaxation occurs by the introduction of misfit dislocations and growth follows a Frank-van der Merwe mode. The formation of an alloy wetting layer is a crucial factor in determining not only how strain is relaxed, but also in influencing the composition, strain gradient and morphology of dots which form from it. In this paper we will present results from in-situ RHEED and STM and ex-situ TEM and STEM measurements and suggest an alternative concept for the origin of dots based on surface structure. Dramatic changes in the morphology, composition and strain state of dots occur during the growth of GaAs confinement layers and we will show how these changes can be monitored by RHEED, AFM, TEM and STEM. There is as yet no adequate model to explain the rate and magnitude of the mass transport processes involved, but we will provide some qualitative suggestions.

2:00 PM ***K4.2**

2-D PRECURSORS AND INTERDIFFUSION IN CdSe/ZnSe SELF ASSEMBLED QUANTUM DOTS. M. Dobrowolska, Department of Physics, University of Notre Dame, Notre Dame, IN.

The evolution of CdSe quantum dots on ZnSe was investigated on a series of samples grown by MBE with nominal CdSe coverage ranging from 0.5 to 2.6 monolayers (ML). TEM data for 0.7 and 1ML coverage available in the literature [1] reveal the existence of 2D areas with increased Cd composition. In our study we investigated the 1.5 and 2.6 ML samples by means of the Z-contrast imaging made possible by scanning transmission electron microscopy (STEM). In this technique the contrast in the image strongly depends on the atomic number Z of the atoms in the material. The image observed on the sample with 1.5 ML coverage reveals the co existence of 2D platelets, 3D islands, and of intermediate objects, showing clearly that 2D islands act as precursors for the formation of 3D islands (dots). These images also reveal that the dots extend to the same degree above and below the interface, providing graphic evidence that the interdiffusion plays an important role in the dynamics of quantum dot formation. The macro- and micro-PL results fully confirm the above STEM data. For the coverage below 1.5ML we observe PL emission characteristic of 2D islands; for coverage between 1.5 and 1.9 ML we simultaneously observe emission from both 2D and 3D islands; while in the sample obtained by deposition of 2.6 ML CdSe only emission characteristic of 3D islands is observed. The above STEM and optical data fully support the growth mechanism of self assembled QD predicted by Priester and Lannoo [2].

*This work was carried out in the collaboration with: C.S. Kim, M. Kim, S. Lee, J.K. Furdyna, H. Rho, L.M. Smith, H. E. Jackson, E.M. James, Y. Xin and N.D. Browning
[1] I.L. Krestnikov et al., PRB 60,8695 (1999).
[2] C. Priester and M. Lannoo, PRL 75, 93 (1995).

2:30 PM ***K4.3**

SELF-ORGANIZATION OF WIDE-BANDGAP II-VI QUANTUM DOTS. Fritz Henneberger, Humboldt Univ of Berlin, Berlin, GERMANY.

This paper addresses the physical processes behind the formation of CdSe/ZnSe quantum dots. Our specific approach is based on the thermally activated reorganization of an initially two-dimensional MBE-grown CdSe film into an array of quantum dots, occurring during growth interruption. In this way, our analysis is free from epitaxial parameters like fluxes, growth rates, etc. Besides RHEED and different ex situ techniques (TEM, Xray, PL), an UHV-AFM

directly slotted to the growth chamber is used for gaining the required information on structure and morphology. The data demonstrate that in contrast to the standard Stranski-Krastanov equilibrium mode - hystereses and regenerative feedback are inherently involved in the quantum dot formation. Long-term AFM experiments reveal robust stability. There is no evidence for (Ostwald) ripening over periods of several 10 days. This is assigned to the existence of an energy barrier for edge detachment, prohibiting the pass into thermodynamic equilibrium. Optical microprobe data demonstrate structure quality and strongly enhanced Coulomb correlation in these nm-sized CdSe quantum dots.

3:30 PM *K4.4

THERMODYNAMICS OF SELF ASSEMBLY: DOTS AND WIRES.
R. Stanley Williams, Hewlett-Packard Labs, Palo Alto, CA.

The growth of strained overlayers of one material on another can lead to the formation of nanocrystalline islands of various shapes and sizes. Under certain conditions, the surfaces of the strained nanocrystals can be a stabilizing factor, which leads to a local minimum in the free energy of the islands and thus a preferred size for each island shape. Because of the strain fields in the substrate, the islands also repel each other rather strongly. For quantum dots, this could lead to a significant amount of ordering of the dots, but for the case of neat Ge islands on Si(001) the finite-temperature size distribution of the dots is too large to allow ordering. It does, however, lead to a shift of the size distributions of the islands. A fundamental understanding of the thermodynamics of islands on surfaces leads both to a better understanding of the shapes that form, and in turn allows one to create purpose-built shapes. This will be illustrated by the self-assembled and -ordered growth of nanowires.

4:00 PM K4.5

DEPENDENCE OF THE STRAIN ON THE SHAPE OF Ge ISLANDS ON Si(001). Chuan-Pu Liu¹, J. Murray Gibson².

¹Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL, ²Materials Science Division, Argonne National Laboratories, Argonne, IL.

Strain has a tremendous effect on the morphology of coherent Ge islands on Si substrates, but the strain of Ge islands were less studied than the morphology, making the understanding of island growth difficult. In this paper, we measure strain in Ge islands as a function of aspect ratio ranging from 0.1 to 0.2 using a two-beam dark-field diffraction condition in transmission electron microscopy (TEM). The native oxide formed on top of islands is water soluble. By removing the oxide several times in water, we intentionally alter the aspect ratio of Ge islands and so strain can be measured with a full range of aspect ratio. We show a nice linear relationship between strain and aspect ratio. The discrepancies between the experiment and theory are discussed.

4:15 PM K4.6

STABILITY OF ENSEMBLES OF Ge/Si(100) COHERENT ISLANDS. Yangting Zhang, Jeff Drucker, The University of Texas at El Paso, Materials Research Institute, El Paso, TX; M.R. McCartney, D.C. Chandrasekhar, David J. Smith, Arizona State University, Center for Solid State Science, Tempe, AZ.

We have investigated the stability of ensembles of Ge/Si(100) coherent islands by annealing at their growth temperature. Islands grown by molecular beam epitaxy at temperatures of 450, 550, 600 and 650 deg C were annealed for times between 5 and 120 minutes. Small hut clusters, bound by {105} facets appear to be extremely stable structures, surviving the longest anneals with no apparent coarsening. Dome clusters, however, coarsen and we believe that this coarsening is related to Si interdiffusion into the Ge clusters. Large alloyed hut clusters, apparent in as-grown samples only for growth temperatures greater than 600 deg C, appear during annealing at 550 deg C. During anneals at 600 and 650 deg C, we observe novel coarsening behavior leading to arrays of crystallographically oriented alloyed hut clusters resulting from the dissolution of large, alloyed dome clusters.

4:30 PM K4.7

Si_xGe_{1-x} ISLAND FORMATION BY POST-GROWTH ANNEAL ON SUPERCRITICAL LAYERS GROWN BY RPCVD.
K. Grimm^{1,2}, L. Vescan¹, L. Nanver², C.C.G. Visser² and H. Lueth¹.
¹Institute of Thin Film and Ion Technology, Research Centre Juelich, Juelich, GERMANY; ²Laboratory of ECTM, DIMES, TU Delft, THE NETHERLANDS.

The epitaxy of SiGe by CVD has proven itself in the industrial production of semiconductor devices, in particular SiGe HBTs. But also in optoelectronics, both strained and relaxed SiGe are being investigated for use in a variety of applications such as emitters, detectors and waveguides. Knowledge of the growth kinetics of these layers is very important for understanding and controlling the

relaxation mechanisms. This paper presents a study of the relaxation mechanisms for SiGe epitaxy performed by reduced pressure and low pressure CVD. The samples were grown at temperatures from 500 - 700°C and pressures from 0.12 - 40 Torr, with SiH₂Cl₂ and GeH₄ as precursor gasses. The properties of the layers have been investigated by AFM, SIMS, PL and RBS. In contrast to the situation for MBE, we found that under RPCVD conditions the relaxation by 3D-growth (Stranski-Krastanow-growth) was strongly suppressed. Relaxation then occurred by the development of misfit dislocations even in the case of high Ge-concentrations (>40%). This behaviour is attributed to the presence of surfactants such as hydrogen or chlorine, which reduce the surface mobility of the adsorbed species. In-situ annealing experiments led to elastic relaxation by the formation of surface undulations as well as SiGe islands. Due to their formation process these islands reveal a very narrow size distribution and have a high packing density compared to as-grown islands. Thus these island layers show strong photoluminescence. The characteristics of light emitting diodes using them as an active recombination region will be presented.

4:45 PM K4.8

LATERAL STRAIN VARIATION AND ORDERING IN SiGe/Si HUT CLUSTER MULTILAYERS. Frank Flack, Katerina Moloni, Don Savage, M.G. Lagally, University of Wisconsin, Dept of Material Science, Madison, WI.

The growth of self-assembling quantum dot systems by the Stranski-Krastanow epitaxial growth mode are currently the focus of a great deal of intensive research. One aspect of these structures which has proven extremely interesting is their tendency to order both vertically and laterally when grown in multilayers. This is accomplished by the transmission of strain through the intermediate spacer layers. Control of the details of this ordering potentially allows the growth of 3D arrays of quantum dots for uniform charge storage in memory devices or narrow linewidths for quasi-zero-dimensional optical applications. This ordering is most pronounced in the Silicon-Germanium system. We present the results of an AFM study of the evolution of lateral ordering in SiGe/Si hut cluster multilayers grown by UHV-CVD. We primarily study the effects of variance in spacer layer growth temperature and thickness on the communication of strain between layers. By fixing carbon nanotubes to AFM tips, we are able to easily resolve features in the sub-5 nm range granting significantly improved clarity. This increased resolution allows us to view structural details not previously seen. We use this new information to propose models of island nucleation and growth on substrates with laterally inhomogeneous strain distributions to the end of improving control over the island ordering.

SESSION K5: POSTER SESSION

Chairs: Joanna Mirecki Millunchick and Eric D. Jones
Tuesday Evening, April 25, 2000
8:00 PM
Salon 1-7 (Marriott)

K5.1

QUANTUM DOT GROWTH IN THE Si-Ge-C SYSTEM THROUGH MULTI-STEP PROCEDURE. Y. Wakayama, G. Gerth, P. Werner, Max-Planck Institute of Microstructure Physics, Halle, GERMANY; L. Sokolov, Science Academy of Russia, Novosibirsk, RUSSIA.

Our main purpose is to investigate a new technique to grow Ge dots on Si(001) substrates. As a presupposition for the application of quantum dots in the Si-Ge system, the size of the Ge islands should be around 10nm in diameter. Additionally, high size uniformity and high density of the Ge dots are strictly required. However, the Ge dot growth on the Si substrate shows a complex behavior. Concerning the morphology of islands, following three shapes are formed simultaneously on the Si substrate through self-assembly processes: so-called hut, pyramid and dome structures. To overcome this problem and to generate a dominant formation of one of these kinds, we investigated a multi-step procedure, which combines changes of substrate temperature and incorporation of carbon (C) during the growth. For example, the following procedure was studied: i) Ge deposition on Si substrates at low temperature, ii) sub-monolayer C deposition on the surface of the Ge films and iii) post-annealing after Ge and C deposition. Morphologies of thereby prepared specimens were examined by atomic force microscopy and transmission electron microscopy. The structure of Ge deposited at low temperature was characterized as a two-dimensional film. On the one hand, a post-annealing of such films yielded a drastic morphological change. On the other hand, a deposition of a small amount of C on the Ge surface (C thickness ≪ one monolayer) was found to prevent such structural modification. By optimizing experimental conditions, including deposition temperature of Ge, the thickness of C layer and post-annealing temperature, we successfully formed 10nm-sized Ge

islands with high number density. Furthermore, such Ge dots showed high size homogeneity. We will discuss the effect of each procedure on the Ge dot formation and describe various recipes for the Ge dots preparation through multi-step procedure.

K5.2

ATOMIC FORCE MICROSCOPY STUDY OF SELF-ASSEMBLED $\text{Si}_{1-x}\text{Ge}_x$ ISLANDS. Kuo-Jen Chao, Charles Evans and Associates, Sunnyvale, CA; Abul E. Kabir, National Semiconductor, Santa Clara, CA; Rashid Bashir, School of Electrical and Computer Engineering at Purdue University, W. Lafayette, IN.

Self-assembled $\text{Si}_{1-x}\text{Ge}_x$ islands were studied using atomic force microscopy (AFM). The self-assembled $\text{Si}_{1-x}\text{Ge}_x$ islands were formed by a two step process. First highly strained $\text{Si}_{1-x}\text{Ge}_x$ thin films (with $x \sim 0.4$) were selectively grown on a silicon wafer by chemical vapor deposition at 650°C , followed by annealing at 750°C . The size and distribution of the islands was found to be a function of the annealing conditions and an ordered pattern could be achieved with specific annealing conditions. This growth process shows a new way of creating ordered islands (maybe quantum dots) for optical and electronic applications on silicon based devices.

K5.3

FORBIDDEN ZONE MODEL FOR ISLAND SPATIAL DISTRIBUTION IN MOLECULAR BEAM EPITAXY. Vladimir Trofimov, Inst of Radioengineering & Electronics of RAS, Dept of Nanoelectronics, Moscow, RUSSIA.

In the past decade, the spatially self-organized growth during self-assembled quantum dots formation has attracted an appreciable attention. We propose here an forbidden zone model for island space distribution based on our model [1], developed earlier within a familiar Kolmogorov statistical approach. According to the model, every nucleated island acts as an effective sink for migrating adatoms so that around an island there exist an exclusion zone of a some width L within which nucleation is forbidden while outside this zone nucleation proceeds in a usual spatially random manner. Assuming that islands nucleate at random points of an uncovered substrate with a constant intensity and grow at a constant linear rate we derive an exact formula for the probability $W(0,t)$ that an arbitrarily chosen surface region of a some area S at any given time t will be empty (free of islands). Probability $W(0,t)$, calculated with this formula, with increasing L deviates more and more of that calculated with a Poisson formula, describing a random island space distribution. Thus, a simple introduction of the forbidden zone leads to a some ordering degree in a spatial island distribution similar to that observed in experiments. By comparison of the model with experimentally measured island spatial distribution, the model parameter L taking into account phenomenologically the surface strain field effect on a heteroepitaxial nucleation and growth process, can be evaluated. 1. V.I. Trofimov, V.A. Osadchenko, Growth and Morphology of Thin Films, Moscow, Energoatomizdat, 1993, 272pp.

K5.4

3D InAs DOTS AND WIRES ON InP(001). Haeyon Yang, J.B. Smathers, P. Ballet, C.L. Workman and G.J. Salamo, Physics Department, University of Arkansas, Fayetteville, AR.

We report on the formation and evolution of InAs 3D islands on an InP(001) surface using a combined molecular beam epitaxy (MBE) and scanning tunneling microscopy (STM) facility. An InP buffer layer is grown on an InP(001) substrate using a solid source phosphorous. The InAs islands are produced on the InP surface by (i) direct deposition of In and As or by (ii) exchange of P-atoms on the surface with As-atoms. Wires of ~ 1 micrometer length and ~ 3 nm height are observed if the substrate is quenched immediately after the InAs deposition. Wires with similar dimensions are also observed to result from exposure of the InP surface to As_4 . The wires produced by P/As exchange are considered to transform to dots higher than 4nm when the substrate is annealed without As_4 flux. STM images show that the wires have a trapezoid cross-section while islands have a truncated pyramid shape with a 40 nm base. Atomic resolution of dimer rows on top of these 3D islands reveal that the top surfaces are atomically flat. Unlike the case of InAs on GaAs, the top surface of the 3D islands, either wires or islands, form 4×2 surface reconstruction which is the same as seen on the wetting layer.

K5.5

CADMIUM INDUCED MORPHOLOGY CHANGE AND QUANTUM DOT FORMATION IN MOLECULAR BEAM EPITAXY OF ZnO. Yefan Chen, Hang-ju Ko, Soon-ku Hong, Takashi Hanada and Takafumi Yao, Institute for Materials Research, Tohoku University, Sendai, JAPAN; Yusaburo Segawa, PhotonDynamics Research Center, Institute for Physical and Chemical Research, Sendai, JAPAN.

One of the wide band-gap semiconductors, ZnO, has emerged to gain

increasing attention because of its unique optical properties, especially the large exciton binding energy (60 meV), which may be applied to practical low threshold excitonic semiconductor laser diodes in the short wavelength range. Recently, we have developed plasma assisted molecular beam epitaxy [1], to grow single crystal ZnO thin films on sapphire substrate. Room temperature stimulated emission and lasing dependent on excitonic processes have been observed [2]. To approach the real device structures, we try to incorporate Cd into ZnO for bandgap tuning to narrower range. Because CdO has rocksalt structure and the vapor pressure of Cd is much higher than Zn, we found at the growth temperatures higher than 400°C , serious segregation of Cd occurs, which results in the very low incorporation rate at these temperatures. Meanwhile, Cd induced 3×3 surface reconstruction of ZnO is observed even at these high growth temperature. Cd induced change of nucleation size is also observed. The atomic force microscopy investigations show that the morphology of (Cd, Zn)O epilayer featured by hexagonal islands with smooth top surfaces and average diameter of $3 \mu\text{m}$, which is much larger than that of the ZnO epilayer without Cd. No depression is observed on these hexagonal islands indicate that they are not from the screw dislocation induced spiral growth. At low growth temperatures, single layer or fractional layer Cd is incorporated into ZnO, which is finely controlled by reflection high-energy electron diffraction intensity oscillation. The inserted Cd causes the formation of quantum dot like structure. Structural and optical studies on these Cd induced quantum dots will be reported.

K5.6

EXPERIMENTAL EVIDENCE FOR A KARDAR-PARISI-ZHANG DESCRIPTION OF SURFACE MORPHOLOGY DYNAMICS IN GaAs MOLECULAR BEAM EPITAXY. Anders Ballestad, Martin Adamcyk, Tom Pinnington, Tom Tiedje,* Advanced Materials and Process Engineering Lab Department of Physics and Astronomy *also Department of Electrical and Computer Engineering, University of British Columbia, Vancouver, BC, CANADA.

We have investigated the evolution of GaAs surface morphology during thin film growth by molecular beam epitaxy (MBE) on planar and textured substrates. The surface structure is measured during growth with light scattering and after growth by AFM. We find that the surface evolution is stable, and that the mounding commonly observed on GaAs surfaces results from roughness in the starting surface caused by thermal cleaning. Hydrogen cleaned substrates with small amplitude roughness were found to roughen without mounding, confirming that the mounds are not due to unstable growth. We find that the smoothing of initially textured substrates to form shallow mounds is accurately described by an anisotropic version of the Kardar-Parisi-Zhang (KPZ) equation:

$$\frac{\partial h}{\partial t} = \nu \frac{\partial^2 h}{\partial x^2} + \lambda/2 \left(\frac{\partial h}{\partial x} \right)^2 \quad (0.1)$$

as observed in AFM images of GaAs buffer layers. These mounds can be fitted by inverted parabolas separated by cusps (slope discontinuities) as expected from the second order non-linear term in the KPZ equation. Although the second order term is not conservative, the observed parabolic mounds are not consistent with the fourth order conservative non-linear term that is commonly considered in MBE growth models. In this case the mounds would have a fourth order (quartic) shape. An explanation for the apparently unphysical quadratic non-linear term will be presented. The ν parameter in the KPZ equation is found to increase with temperature while the λ parameter decreases with temperature. The anisotropy increases with decreasing arsenic flux. From measurements of the interface width as a function of time and length scale for GaAs buffer layers grown on H-cleaned surfaces we find the roughness exponent α for GaAs homoepitaxy to be 0.43 and the growth exponent β to be 0.16, in reasonable agreement with numerical studies for the isotropic KPZ equation ($\alpha = 0.38$ and $\beta = 0.24$).

K5.7

SELF-SIMILAR GROWTH OF A COMPOUND LAYER IN THIN-FILM BINARY DIFFUSION COUPLES. Huifang Zhang, Harris Wong, Louisiana State Univ, Dept. of Mechanical Engineering, Baton Rouge, LA.

Diffusion controlled growth of a compound phase AnB between two parallel thin films of material A and B is important in electronic materials processing and in synthesis of high-temperature materials using multilayer films. Previous models of the growth rate do not solve the diffusion equation, and thus do not utilize fully the predictive capability. This talk presents a self-similar solution of the diffusion equation with the nonlinear Kirkendall effect included. The nonlinear partial differential equation is converted into a nonlinear ordinary differential equation with a free boundary and solved iteratively by a shooting method. It is found that the intrinsic diffusion coefficients of A and B in AnB are simultaneously determined from the positions of

the interfaces without using the concentration profile in the compound phase. An asymptotic analytic solution valid for small differences in the equilibrium interfacial concentrations is obtained and agrees with the numerical results in the appropriate limit. Implications of this complete solution will be discussed.

K5.8

UNIFORMITY CONTROL ACROSS 5x6 INCH AlGaAs/GaAs AND 35x2 INCH AlGaInP MQWs GROWN IN A PLANETARY REACTOR[®]. [Thomas Schmitt](#), M. Deufel, G. Strauch, D. Schmitz, M. Heuken, H. Juergensen, Aixtron AG, Aachen, GERMANY.

To meet industrial requirements we developed the Planetary Reactor[®] with the capability to grow simultaneously on 5x6 inch wafer. Growth was carried out at 100 mbar and a H₂ carrier gas flow of typical 24 sl/min which results in the very low specific epi area flow of 0.17 l/(min.sqin). Uniformity optimisation for the 5x6 inch configuration was carried out by appropriate control of the carrier gas flow certainly trying to keep consumption as low as possible. The group III efficiency also improves from 40% to 54% by decreasing the total flow to 17 sl/min. Nevertheless, the optimum thickness uniformity of $\pm 0.5\%$ is obtained at 24 sl/min with a group III efficiency of about 50%. Further finetuning of hardware and growth temperature allows maximum precursor efficiency at this point as high as 54% with equal thickness uniformity. The control of thickness uniformity was tuned using sensitive 5x6 inch AlAs/GaAs DBR (Distributed Bragg Reflectors) which show an average reflected wavelength of 552.4 nm and an overall standard deviation of 3.1 nm which is 0.5%. Silicon doped GaAs on 6 inch wafer show a standard deviation of the sheet resistance of 0.85% at a carrier concentration of $1.1 \times 10^{18} \text{cm}^{-3}$ and a mobility of 1600 cm²/Vs. Intrinsic carbon doping show sheet resistance uniformities of 3.7%. AlGaAs (x = 0.28) composition uniformity was checked by photoluminescence and X-ray mapping. We routinely obtain a standard deviation of emission wavelength of 0.5% across a full 6 inch wafer. Finally we show equal performance of AlGaInP/AlGaInP multi quantum wells grown on a satellite with one 6 inch and a satellite with 7x2 inch wafer. At the selected mean emission wavelength of these MQW of 616 nm, the maximum to minimum wavelength deviation from the mean wavelength is $\pm 2\text{nm}$.

K5.9

UNIFORMITY CONTROL OF 3 INCH GaN/InGaN LAYERS GROWN IN PLANETARY REACTORS[®]. [Mike Bremser](#), Aixtron Inc, Pasadena, CA; [H. Protzmann](#), M. Luenenbuerger, M. Heuken and H. Juergensen, Aixtron AG, Aachen, GERMANY.

We present results obtained from a 2400G3HT reactor with a maximum wafer capacity of 8x3 inch. To achieve uniformity of the growth, we increased the temperature uniformity on each satellite to 0.9°C and from satellite to satellite to 0.8°C. The optimum reactor geometry has been found by extensive modeling of the reactor design. Thus an optimization of uniformity and efficiency has been achieved. GaN, InGaN/GaN-MQW, GaN:Si, GaN:Mg and AlGaIn was obtained on 5x3 inch substrates by simple scaling of the corresponding process parameters of the 6x2 inch configuration. The group III precursor efficiency could be kept at about 17%. We will demonstrate GaN:Si and GaN:Mg doping uniformity with a standard deviation of less than 5% with thickness uniformities of less than 7% standard deviation without any edge exclusion. Considering a 3mm rim, the thickness uniformity is in the range of 3-4%. InGaN/GaN quantum well emission at 480 nm shows a standard deviation of 3-4 nm without rim exclusion. We grew AlGaIn with about 10% Al content and less than 2% standard deviation in Al composition across the 3 inch substrate. Simple electroluminescence test structures, consisting of a GaN:Si buffer, followed by a 5 period InGaIn/GaN quantum well and covered by a GaN:Mg cap with emission wavelengths of about 460 nm show wavelength variations across 3 inch wafers of less than 3nm. All these results demonstrate that the AIXTRON Planetary Reactor is a very flexible tool for mass production application, especially with respect to upgrading the system to larger wafer diameters as already well known from the standard GaAs and InP application which are available up to 5x8 inch configurations.

K5.10

NANOWIRES FROM VAPOR CONDENSATION AND THEIR ASSEMBLIES. [Yiyang Wu](#), [Franklin Kim](#), [Benjamin Messer](#), [Michael Huang](#), [Peidong Yang](#), Department of Chemistry, University of California, Berkeley, CA.

Chemical vapor transport and deposition in both open-tube and sealed-tube system was used to synthesize single crystalline semiconductor (Ge, Si) and oxide nanowires. These nanowires were grown through the vapor-liquid-solid process. Their diameters are in the range of 5 -100 nm depending on different sizes of metal cluster catalysts (Au, Fe) we use and can be hundreds micrometer long. In addition, Nanowire arrays were grown from patterned metal catalysts fabricated using optical lithography or soft lithography techniques.

The surface of these wires were further chemically functionalized and their assembly chemistry in solution will be presented.

K5.11

STRUCTURE AND OPTICAL PROPERTIES OF InAs INSERTIONS IN A SILICON MATRIX FORMED BY MOLECULAR BEAM EPITAXY. [Nikolai D. Zakharov](#), [P. Werner](#), [U. Gosele](#), Max-Planck Institute of Microstructure Physics, Halle/Saale, GERMANY; [R. Heitz](#), [D. Bimberg](#), [N.N. Ledentsov](#), Technical University of Berlin, GERMANY; [V.M. Ustinov](#), [D.V. Denisov](#), [B.V. Volovik](#), [Zh. I. Alferov](#), [A.F. Ioffe](#) Physico-Technical Institute, St. Petersburg, RUSSIA; [G.E. Cirlin](#), Institute for Analytical Instrumentation, St. Petersburg, RUSSIA.

Single and multiple InAs insertions in a Si matrix are grown by MBE on Si (100) substrates and investigated by HRTEM. Ultrathin (sub- and one-monolayer) InAs insertions can be easily formed, as demonstrated by HRTEM. In the case of several monolayer-thick insertions capped with Si and annealed at 800°C, an extensive In-As-Si interdiffusion accompanied by formation of InAs solid solution and domains of ordered InAs-Si phases in a Si matrix is observed. The InAs-rich regions (diameter about 6nm) are distributed in the whole epilayer and composed of alternating InAs and Si planes. Two types of ordering are revealed: (i) the first type shows an ordering of (101), (10 $\bar{1}$) planes inclined to the [001] growth direction, while in the second type (ii) the ordered (110) planes are parallel to [001] growth direction. Formation of such ordered structures, presumably, results in energy reduction caused by a decreased number of mixed Si-As and Si-In bonds. We also found that the samples containing InAs solid solution in Si and InAs-rich domains demonstrate a broad photoluminescence peak in the 1.3 μm range. We attribute this luminescence to the local band gap narrowing resulting from the formation of the solid solution and/or the nanodomains.

K5.12

FORMATION OF SELF-ASSEMBLED NANOMETER-SCALE InP ISLANDS ON SILICON SUBSTRATES. [Andrey S. Bakin](#), [Dirk Piester](#), [Hergo-Heinrich Wehmann](#), [Alexei A. Ivanov](#) and [Andreas Schlachetzki](#), Institute for Semiconductor Technology, Technical University of Braunschweig, Braunschweig, GERMANY.

Self-assembled nanometer-scale structures are at present topics of considerable interest due to their potential in optoelectronic and electronic device application. The heterostructures of direct band-gap material as InP on indirect band-gap silicon are of great interest for a new generation of optoelectronic devices monolithically integrated with silicon microelectronics. Three-dimensional islands of InP have been reproducibly grown in the Stranski-Krastanow (SK) growth mode on Si (001) and (111) by using metal-organic vapor phase epitaxy (MOVPE). Atomic-force microscopy (AFM) was used to determine the morphology of the samples and to evaluate the dimensions of the islands. The growth was performed in a horizontal infrared-heated MOVPE machine designed by AIXTRON and operated at low pressure (20 to 100 hPa). Prior to growth the wet-chemically cleaned Si substrates were thermally treated in a hydrogen atmosphere to remove the native oxide. Arsine was introduced during the cool-down phase and then growth was started at 400°C. Using the same optimized growth conditions samples with different InP islands were obtained by variation of the growth duration. AFM revealed the formation of three-dimensional islands with densities as high as 10^{10}cm^{-2} . In order to investigate the effect of annealing, the samples with different densities of nanoscale three-dimensional islands, obtained as described above, were heated in phosphine flow up to the temperature of 640°C. Then the morphology of the samples has been studied. The results obtained are explained in terms of strain-relaxing mechanisms at the first stages of InP/Si heteroepitaxy. The formation of gradually relaxing three dimensional islands over a fully strained initial two-dimensional wetting layer through a growth mode transition at the initial stages of heteroepitaxial growth is discussed. It is shown that MOCVD provides an excellent control over growth rates down to a few monolayers coverage.

K5.13

FORMATION OF CONTINUOUS NANOMETER PtSi THIN FILM ON Si BY PULSED LASER DEPOSITION(PLD). [Meicheng Li](#), School of Materials Science and Engineering, Harbin Institute of Technology, Harbin, CHINA; [Xuekang Chen](#), [Jing Wang](#), [Jianping Yang](#), [Zhanxu Lei](#), [Gan Wu](#), Lanzhou Institute of Physics, Lanzhou, CHINA; [Liancheng Zhao](#), School of Materials Science and Engineering, Harbin, CHINA.

Metal based silicides on silicon substrates are a widely used material system for infrared detection. PtSi/p-Si infrared Schottky barrier detectors (IRSBD) have become one of the most successful photoemissive infrared detectors. Till now, most of the efforts have been focused on the design of two dimensional PtSi-SBD arrays for

the infrared (IR) camera. In this paper we discussed the formation condition of PtSi and their effects on the Schottky barrier potential. PtSi films at different preparing conditions are compared, including different annealing sequences, annealing time, film thickness, and annealing ambients using pulsed laser deposition on various temperature substrates. Film structures and compositions, phases formation, and Schottky barrier potential using different processes are analyzed. By studying the kinetics of PtSi formation during various annealing processing, preferable preparing conditions are proposed to form the continuous PtSi ultra-thin film on Si substrate by PLD.

K5.14

EFFECT OF COPPER-INDUCED RECRYSTALLIZATION ON THE PIEZORESISTIVITY OF GERMANIUM FILMS. A. Khakifirooz, S.S. Mohajerzadeh, S. Haji and E. Asl Soleimani, University of Tehran, Electrical and Computer Eng. Dept., Tehran, IRAN.

It has been shown that the crystallization of germanium can be mediated by the incorporation of copper. This is believed to be due to the formation of copper germanide, which acts as a nucleation seed for Ge [1]. In this paper, we report the effect of metal-induced crystallization (MIC) on the piezoresistivity of Ge films. Polycrystalline Ge films with a thickness of 1000 Å are e-beam deposited on a 50 μm thick glass substrate at 400°C, followed by evaporating 100 Å of Cu on some of the samples at room temperature. These samples are then vacuum annealed at 400°C for 30 minutes. SEM, XRD, RBS, and PIXE were used to examine the crystal structure and composition of the films. In addition to the formation of Cu₃Ge, XRD analyses show a significant growth of the grain size and a dominant Ge(111) orientation, whereas both (111) and (220) orientations have similar importance in as-grown Ge films. The preference of (111) orientation is also observed in amorphous films recrystallized by MIC. For the purpose of electrical measurements, Cu₃Ge and remaining copper are etched away using phosphoric acid and devices are then fabricated by photolithography. Hall measurements show that MIC causes the hole mobility to increase from 25 cm²/V.s to about 77 cm²/V.s, while cantilever bending indicates that longitudinal and transverse gauge factors change from 32 and -16 to 57 and -14, respectively. The larger longitudinal sensitivity is a result of the grain size growth, while the higher anisotropy may be attributed to the dominant (111) orientation [2]. With the addition of silicon into Ge films, we expect to achieve polycrystalline SiGe films on glass substrates using a similar MIC technique. The research on making thin film transistors using SiGe films is underway. References: [1] J.P. Doyle, et al., Appl. Phys. Lett., 67, p. 2804, 1995. [2] P. Ciureanu and S. Middelhook, Thin Film Resistive Sensors, IOP Publishing, London, 1992.

K5.15

EVOLUTION OF SURFACE MORPHOLOGY AND EPILAYER TILT IN HIGHLY MISMATCHED InSb FILMS. X. Weng, R.S. Goldman, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI; D.L. Partin, J.P. Heremans, Delphi Research and Development Center, Warren, MI.

InSb is useful for a wide variety of device applications, including long wavelength infrared sources and magnetoresistive sensors. InSb films are often grown with a 14.6% lattice mismatch on GaAs substrates. Because of the high mismatch, InSb films generally grow in a Volmer-Weber mode, which consists of nucleation and coalescence of three-dimensional islands. However, the evolution of the surface morphology and the epilayer rotation about an in-plane axis (epilayer tilt) in highly mismatched systems is not well understood. Therefore, we have investigated the evolution of surface morphology and epilayer tilt in 0.1 to 1.5 μm thick InSb films grown on GaAs substrates. High resolution X-ray diffraction (HRXRD) measurements indicate that these films are not fully relaxed and that the residual strain decreases with increasing film thickness. Atomic force microscopy (AFM) and cross-sectional transmission electron microscopy (TEM) show that the 0.1 μm films consist of coalesced islands with a ratio of root-mean-square surface roughness (R_{rms}) to film thickness of ~5%. This ratio drops to a nearly constant value of ~1% for films with thicknesses beyond 0.2 μm. Both the orientation of surface features and epilayer tilt axis rotate about the surface normal as the film thickness increases. Initially, the magnitude of tilt increases with film thickness, thereby decreasing the offset. For 0.55 μm films, the tilt magnitude begins to decrease, suggesting the presence of reverse tilt, where the tilt increases the offset. In lower misfit systems, this type of tilt reversal has been correlated with the presence of surface facets which generate local offsets. We have also studied the microstructure of the InSb/GaAs interface using high resolution transmission electron microscopy (HRTEM), and find the coexistence of pure edge and 60° misfit dislocations at the interface. The interplay between interfacial dislocations, residual strain, epilayer tilt, and surface morphology will be discussed.

K5.16

INFLUENCE OF GROWTH TEMPERATURE AND PHOSPHINE FLOW ON CuPt TYPE ORDERING IN InGaP GROWN BY CHEMICAL BEAM EPITAXY. J. Bettini, M.M.G. de Carvalho, M.A. Hayashi, L.P. Cardoso, Dept of Applied Physics/UNICAMP, Campinas, SP, BRAZIL; D. Ugarte, LNLS/MCT, Campinas, SP, BRAZIL.

In this work, we present a study on ordering of InGaP layers grown by Chemical Beam Epitaxy (CBE) on (100) GaAs substrates. The samples were grown at temperatures in the range 500-560°C and phosphine flow between 5-40 sccm. In all samples, growth parameters were chosen in order to keep the InGaP layers lattice matched to the substrate. Transmission Electron Diffraction shows CuPt type ordering in all samples. Only in the most ordered samples, ordering can also be seen by X-Ray Diffraction. A reduction in the band gap energy is observed with 77K photoluminescence measurements and associated to the ordering in the InGaP layer. Transmission Electron Microscopy dark field was utilized to study size and density of the ordered regions as a function of growth parameters (growth temperature and phosphine flow). In the range of temperature considered here, we have observed that the density and size of the ordered regions increase with growth temperature, but do not attain the same degree of ordering attained by Organometallic Vapor Phase Epitaxy (OMVPE) technique. The greater ratio between ordered/disordered area is about 30% for our samples, nearly one half of this same ratio for sample obtained OMVPE. The higher value of this ratio in our case occurs at growth temperature of 560°C. At higher growth temperature, it becomes very difficult to keep the lattice-matched composition in the layers grown by CBE. So ordering degrees as high as those obtained by OMVPE, as well as the maximum ordering temperature, can not be reached using CBE. In this sense, we have always observed higher degrees of ordering with increasing growth temperature. Our results can thus explain why in CBE gap reduction is observed when growth temperature is increased. Phosphine flow appears to mainly have influence in the size of these regions.

K5.17

EFFECT OF LATTICE MISMATCH ON THE DECAY OF RHEED OSCILLATIONS DURING GROWTH OF STRAINED InGaAs/GaAs HETEROSTRUCTURES. Akos Nemcsics, Ferenc Riesz.

The decay of the oscillation of the reflection high-energy electron diffraction pattern is analyzed during the molecular beam epitaxial growth of strained InGaAs/GaAs heteroepitaxial structures. The oscillations' amplitude was found to decrease exponentially versus time during the InGaAs growth. Further, the decay time constant decreases exponentially with InAs mole fraction, indicating that the lattice strain increases islanding during growth. A quantitative model based on the growth front roughening is formulated to explain the results. Assuming that the oscillation decay is related partly to the strain and partly due to kinetic effects during growth, a decay component that is solely due to strain is separated. We find that onset of increased roughening due to misfit strain component corresponds to the Matthews-Blakeslee critical layer thickness.

K5.18

CHARACTERISATION OF MORPHOLOGY AND DEFECTS IN SILICON-GERMANIUM VIRTUAL SUBSTRATES. Gabriela D.M. Dillway, Arthur F.W. Willoughby, Materials Research Group, School of Engineering, University of Southampton, Southampton UNITED KINGDOM; Janet M. Bonar, Department of Electronics and Computer Science, University of Southampton, Southampton, UNITED KINGDOM.

Silicon-germanium heterostructures incorporating virtual substrates are successfully used for both microelectronic and optoelectronic applications. However, their use may be limited by their rough surface morphology and high threading dislocation density. This work reports the effects of the growth parameters on the morphology and defects in SiGe virtual substrates grown by Low Pressure Chemical Vapour Deposition (LPCVD). Structures with a graded Ge composition region followed by a constant Ge composition region were grown on 4-inch (001) Si substrates by LPCVD using H₂, SiH₄ and GeH₄. Growth parameters varied included Ge gradient (stepwise or linear change), growth temperature, and capping layer thickness. The samples were characterised by Nomarski Differential Interference Contrast (DIC) Microscopy, Transmission Electron Microscopy (TEM) and Atomic Force Microscopy (AFM). All samples exhibited periodic undulations of the surface along perpendicular <110> directions (cross hatch pattern) when imaged in Nomarski contrast. In the linear graded structures, cross-section TEM observations showed dislocation pileups terminating in trenches. In conjunction with AFM observations, examination of the dislocations in cross-section TEM led to the conclusion that the linear-graded structures were relaxing through a surface roughening mechanism, which is accentuated at higher growth

temperatures. The linear graded structures were found to have Root Mean Square (RMS) surface roughness of 20–40 nm, while the step graded structure appeared superior with a significantly lower RMS at 5–7 nm. The virtual substrates grown by this LPCVD technique have thus been shown to be comparable to those grown by other methods.

K5.19

THE GROWTH OF HIGH QUALITY GaAs EPILAYERS ON STRIPE PATTERNED InP SUBSTRATES WITH A TRANSFERRED GaAs FUSED LAYER. Sung Min Hwang, Ju Young Lee, Eun Kyu Kim, Semiconductor Materials Laboratory, Korea Institute of Science and Technology, Cheongryang, Seoul, KOREA; In-Hoon Choi, Department of Material Engineering, Korea University, Anamdong, Sungbukku, Seoul, KOREA; Yong Kim, Department of Physics, Donga University, Pusan, KOREA.

Recently, the heteroepitaxy for onto electronic device is very actively being investigated, especially in the field of hetero junction between GaAs and InP is dynamically being studied. In this work, we performed the growth of high quality GaAs epi-layer on InP substrates using the wafer fusion method. The fused GaAs epi-layers were patterned by a stripe line. Then a consequent overgrowth of GaAs was executed using the atmosphere metal-organic chemical vapor deposition (AP-MOCVD). As the results of micro-photoluminescence (μ -PL), scanning electron microscopy (SEM), and atomic force microscopy (AFM), it was observed abnormal growth morphology causing the reduction of lateral growth rate. In spite of 3.8% lattice mismatch, we could check the bound exciton signal of GaAs epi-layers peaked at 824 nm with full width at half maximum (FWHM) of 6 meV at 77 K. These results represents a significant improvement of the optical property compared to the previous reports related with the GaAs epi-grown on InP substrate. Also, we can observe a dramatic difference in surface morphology between the growth using our method and a conventional GaAs/InP growth through an AFM measurement.

K5.20

SELECTIVE CONTROL OF InAs SELF-ASSEMBLED QUANTUM DOTS ON GaAs WITH SUB-MICRON METAL PATTERNS. Maeng Ho Son, Bum Ho Choi, Chan Kyeong Hyon, Eun Kyu Kim, Semiconductor Materials Laboratory, Korea Institute of Science and Technology, Cheongryang, Seoul, KOREA; Yong Kim, Department of Physics, College of Natural Sciences, Donga University, Pusan, KOREA; Jong Soo Lim, Department of Physics, Kyonggi University, Yui-Dong, Suwon, KOREA; Seung Taek Lim, Jin Ho Ahn, Department of Metals Engineering, Hanyang University, Hangdang, Seoul, KOREA.

We study the formation of InAs self-assembled quantum dots (SAQDs) on GaAs substrates with sub-micron platinum (Pt) and tungsten (W) metal patterns. In Pt case, an island density reduced region with roughly 2 μ m near the boundary of the pattern is found. However, it is unable to use the quantum devices, because the Pt metal is reaction with AsH₃. So, we suggested that the tungsten (W) would be better candidate to avoid such as reaction. In W case, SAQDs and islands are observed in the non-patterned region between two stripe tungsten metal patterns. On the other hand, an island density reduced region with W pattern is changed by the buffer layer thickness. The width of island density reduced region at the zero and 15 nm buffer layers are approximately 15 nm and 0.4 μ m, respectively. Our observation can be applied directly to a single electron device (SET). In this case, source and drain fingers are fabricated first before SAQD growth. This result may show a possible way for the how to connect electric leads to randomly positioned individual SAQD.

K5.21

ALIGNMENT OF THE InAs QUANTUM DOTS ON GaAs USING THE MANIPULATION OF STRAIN FIELDS. Kwang Moo Kim, Young Ju Park, Young Min Park, Chan Kyeong Hyon and Eun Kyu Kim, Semiconductor Materials Laboratory, Korea Institute of Science and Technology, Cheongryang, Seoul, KOREA; Jung Ho Park, School of Electrical Engineering, Korea University, Anamdong, Sungbukku, Seoul, KOREA.

The site control of the quantum dots (QDs) is crucial for the device applications. The self-assembled growth mode can be controlled by the surface elastic strain energy. Lateral alignment of InAs QDs were investigated by manipulating the strain fields of In(Ga)As/GaAs superlattice (SL). Using molecular beam epitaxy, we firstly formed strained SL structure in order to modify the surface strain energy of GaAs matrix, and then grew the self-assembled InAs QDs on it. The nucleations for the QDs were preferably formed along the $\langle 110 \rangle$ direction. More specifically, the trend of two-dimensionally aligned QDs along the $\langle 110 \rangle$ showed an anisotropic morphology. The density and size of QDs along the $[110]$ were higher and larger than those along the $[1\bar{1}0]$. This indicates that the anisotropic alignment of QDs are closely related with the occurrence of misfit dislocation due

to the critical thickness of lattice relaxation. On the basis of calculated critical thickness of SL, we formed InAs/GaAs strained layer of superlattice with proper surface elastic strain energy. As a results, we obtained two-dimensionally aligned self-assembled InAs QDs without any patterning process.

K5.22

THERMAL STABILITY OF Si/Ge HETERO-INTERFACE GROWN BY ATOMIC-LAYER EPITAXY. Keiji Ikeda, Jiro Yanase, Satoshi Sugahara and Masakiyo Matsumura, Dept of Physical Electronics, Tokyo Inst. of Technology, Tokyo, JAPAN.

Thermal stability has been evaluated for a hetero atomic-layer-epitaxy (ALE) grown Si layer on Ge(100) [1] by using coaxial impact-collision ion scattering spectroscopy (CAICISS) for the first time. The ALE-grown 2ML-Si/Ge interface was stable up to 550°C. Although CAICISS is said surface-sensitive, its TOF spectrum contains a lot of Ge bulk components, which cover weak components from the topmost Si and/or Ge surface. Thus, at first, we studied a data reduction method, and found that subtracted TOF Spectrum, STS, from the reference spectrum of bulk Ge shows clearly the change of the topmost surface. The sensitivity on the topmost surface change was about 0.2ML. A 1ML-Si layer was grown on Ge(100) by ALE, i.e., in a self-limiting manner by exposing SiH₄ at 310°C. STS indicated that the topmost surface is changed from Ge to Si. The surface H atoms, although they are not detected by CAICISS, effectively suppress the Ge surface segregation by their surfactant effects at these temperatures. Next, a 2ML-Si layer on Ge(100) was grown by ALE, i.e., in a self-limiting manner by exposing a 1ML-Si grown sample to SiH₂Cl₂ at 530°C, STS indicated no surface Ge atom. This is resulted from the fact that Si-precursor has been absorbed on a successively born surface dangling bond within a much shorter incubation time than the Ge atom segregates competitively on the surface. For the ALE-grown 2ML-Si/Ge structure, the Ge surface segregation was not detected upto 550°C. This highly stable feature resulted from a pre-formation of strong Si-Si network in the 2ML-Si layer on the top. In conclusion we have shown that hetero-ALE has a very attractive but different feature compared with MBE or Gas-source MBE that it can form a thermally stable Si/Ge interface. Reference [1] K. Ikeda et al.; Jpn. J. Appl. Phys. 37 (1998)1311.

K5.23

THE EFFECT OF INDIUM SURFACTANT ON THE OPTOELECTRONIC AND STRUCTURAL PROPERTIES OF n-TYPE GALLIUM NITRIDE. Changfei Zhu, W.K. Fong, B.H. Leung, C.C. Cheng and C. Surya, Department of Electronic and Information Engineering, The Hong Kong Polytechnic University, HONG KONG.

GaN films were grown by rf-plasma assisted molecular beam epitaxy. A small In flux was used as a surfactant during the growth of films. The optoelectronic properties of the films grown with and without In surfactant were characterized by investigating the photoluminescence, high resolution x-ray diffraction and low frequency noise power spectra. The sample grown in the presence of In surfactant shows a better photoluminescence spectrum. Especially, the intensity of yellow band emission becomes much weaker. The full width at half-maximum (FWHM) of the (0002) GaN diffraction peak, obtained from x-ray rocking curve, decreased from 0.443deg to 0.352deg when In surfactant was used. The slope of voltage noise power spectral density versus f is very close to the $1/f$ (Flicker noise) for both samples. The value of the Hooge constant is smaller for the sample with In surfactant. These results indicate that the presence of In during the growth of GaN is beneficial for improving the optoelectronic and the structural properties of GaN.

K5.24

DETERMINE THE THREE-DIMENSIONAL CRYSTALLOGRAPHIC MISORIENTATION IN HETERO-STRUCTURES BY SELECTED AREA DIFFRACTION (SAD) IN TEM. X.J. Guo, National Taiwan Univ, Dept of Chemistry, Taipei, TAIWAN; J.H. Huang, National Tsing-Hua Univ, Center for Materials Sciences, Hsinchu, TAIWAN; H.C. Shih, National Tsing-Hua Univ, Dept of Materials Science and Engineering, Hsinchu, TAIWAN.

Interfacial defects are found to be misfit dislocations, microtwins, and stacking faults. These defects are responsible for the random misorientation of the heteroepitaxial diamond films on silicon, heteroepitaxial GaN layers grown on (0001) sapphire, and heterostructures of semiconductors built by direct wafer bonding. In this report, a concise scheme is proposed to determine the crystallographic misorientation of heteroepitaxial structures. In addition to subtle high-resolution transmission electron microscope images, the information revealed from selected-area diffraction patterns at the interfaces offers another path to determine the angles of misorientations. The principle is to extract the basically three-dimensional misorientation information from a two-dimensional

selected-area diffraction patterns through the employment of the Laue circle.

K5.25

STRUCTURE AND OPTICAL CHARACTERISTICS OF AlN AND AlGa_N ALLOYS THIN FILMS. Janis Jansons, Maris Springs, Ivar Tale, Aris Veispals, Institute of Solid State Physics, University of Latvia, Riga, LATVIA; Hans-Joachim Fitting, Heinrich Stolz, Physics Department, Rostock University, Rostock, GERMANY.

The AlGa_N alloys hold promise for developing ultraviolet photo-detectors, MESFET, MODFET, bipolar transistors, light-emitting diodes and laser diodes. Native and introduced defects strongly influence their optical and electronic properties. The optical properties of mono crystalline AlN and AlGa_N thin films grown by MOVPE on sapphire substrates were investigated by transmittance, reflectance, photoluminescence and cathodoluminescence measurements. Epitaxial films were deposited in two step process, with a low temperature buffer layer. The structure of films was tested by X-ray diffraction and scanning microscope techniques. The excitonic absorption edge of AlGa_N alloys continuously shifts from 3.43 eV to 6.2 eV by increase of the Al content in alloy. An additional absorption slope, distinct from the Urbach tail and caused by defects was observed even at Al concentration of some percent. The structured absorption tail below the band edge was detected in films ranging in Al concentration above 55%. The photoluminescence and cathodoluminescence spectra in the whole Al concentration range are represented by exciton related luminescence bands peaked close to the band gap. In films ranging in Al concentration above 60% new luminescence bands peaking in spectral range 2 - 4.5 eV occur. Introduction of oxygen in film results in considerable increase of these luminescence bands. It can be expected that principal presence of deep defects in AlGa_N alloys at high concentration of Al can be an important problem in development of electronic and optoelectronic devices.

K5.26

ANALYSIS OF STRUCTURAL PROPERTIES OF AlGa_N EPILAYER WITH VARIATION OF AlN MOLAR FRACTION. Je Won Kim, Young K. Park, Seong-II Kim and Yong Tae Kim, Korea Institute of Science and Technology, Semiconductor Materials Laboratory, Seoul, KOREA; In-Hoon Choi, Korea University, Dept of Materials Science, Seoul, KOREA.

AlGa_N alloy is a very attractive material to use in UV photo-detectors, high electron mobility transistors, and field-effect transistors, based on AlGa_N/Ga_N heterostructures, holding promise for high power and high-temperature electronics device applications. In order to achieve the bandgap engineering in the heterostructures of Al_xGa_{1-x}N, it is essential to investigate the dependence of structural properties of Al_xGa_{1-x}N as a function of AlN molar fraction (x) and achieve the better control of AlN composition without a compositional fluctuation in depth of the epilayer. In this work, the structural properties of Al_xGa_{1-x}N epilayers grown on (0001) sapphire by molecular beam epitaxy (MBE) with variation of AlN molar fraction is characterized by Auger electron spectroscopy (AES) and atomic force microscopy (AFM).

K5.27

A THEORETICAL STUDY ON DOMAIN BOUNDARIES IN EPITAXIAL WURTZITE GaN FILM. Shaoqing Wang, Hengqiang Ye, Laboratory of Atomic Imaging of Solids, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, PR CHINA.

GaN attracts extensive research interests both in science and in industry for its potential use in the manufacture of photoelectric devices. This paper reports our attempt for a molecular dynamics study on various domain boundary structures in Wurtzite GaN. The domain boundaries can be classified into two types along {1-100} and {11-20} planes in Wurtzite GaN, respectively. Our research results show that the domain formation energies of (1-100) and (11-20) boundaries are significantly different. The latter ones have general quite higher formation energies than the formers. All the like-atom bonding domain boundaries have higher formation energies than their counterparts of unlike-atom bonding domain boundaries in both of GaN (1-100) and (11-20) interfaces. There will be more (1-100) rather than (11-20) domain boundaries in Wurtzite GaN from the viewpoint energetically. This conclusion is in accordance with the usual experimental observations that most grain boundaries are (1-100) boundaries. All the unlike-atom bonding domain boundaries can form stable atom configurations. The atom positions are regular and symmetrical at the boundaries. While most of the like-atom bonding domain boundaries are unstable. The atom positions are irregular and lack of symmetry at the boundaries. A simple way to differ these domain boundaries can be that the atomic images by unlike-atom boundaries will be clearly distinguishable regular-arranged image patterns while the images of like-atom boundaries will contain many irregular patterns and be serious blurred by experiment of high-

resolution electron microscopy. We found one exceptional (1-100) like-atom bonding boundary. Its domain formation energy is not quite high. The boundary configuration is stable and there is no serious lattice distortion. It can not be easily observed by high-resolution electron microscopy.

K5.28

X-RAY PHOTOELECTRON SPECTROSCOPY EVALUATION OF SURFACE CHEMICAL STATES OF GaN, InGa_N AND AlGa_N HETEROEPITAXIAL THIN FILMS GROWN ON SAPPHIRE BY MOCVD. K. Li, Institute of Materials Research and Engineering, SINGAPORE; A.T.S. Wee, J. Lin, National Univ of Singapore, Dept of Physics, SINGAPORE; Z.C. Feng, S.J. Chua, Institute of Materials Research and Engineering, SINGAPORE.

The surface chemical states of MOCVD grown GaN, AlGa_N and InGa_N, and the influence of different dopants have been studied with x-ray photoelectron spectroscopy (XPS). The results show that for most of the samples the N 1s peak can be deconvoluted into a dominant GaN peak at the binding energy of about 397.2 eV and a small N-H peak at the binding energy of about 398.5 eV, while Ga 3d can be deconvoluted into three peaks, ie, elemental Ga at 18.5 eV, GaN at 19.7 eV, and Ga₂O₃ at 20.4 eV. Si-doping appears to change the surface oxidation property of GaN by causing a change of intensities in the relative components of the Ga 3d peak. Compared with Si doping, the influence of Mg-doping appears to be larger. In addition to a change in the component intensities, Mg-doping also causes the N 1s and Ga 3d peaks to broaden. The ternary AlGa_N sample shows the surface segregation of aluminum. For the undoped InGa_N, surface indium deficiency is observed. Due possibly to trapped N-H and Ga-CH intermediate species at grain boundaries, the Zn doped InGa_N sample shows a relatively larger N 1s peak at 398.78 eV and an additional Ga 3d peak at 21.4 eV respectively.

K5.29

FORMATION OF GALLIUM NITRIDE (GaN) TRANSITION LAYER BY PLASMA IMMERSION ION IMPLANTATION AND RAPID THERMAL ANNEALING. Dixon T.K. Kwok, Aaron H.P. Ho, X.C. Zeng, Chung Chan and Paul K. Chu, Department of Physics and Material Science, City University of Hong Kong, Hong Kong, CHINA; S.P. Wong, Department of Electrical Engineering, Chinese University of Hong Kong, Hong Kong, CHINA

Recent advances in the preparation of gallium nitride (GaN) and related compounds have promised the commercial production of blue semiconductor light emitting devices. Typical preparation of GaN involves growing the materials on sapphire or silicon carbide using metal-organic chemical vapor deposition (MOCVD). The lattice mismatch between GaN and the substrate makes it difficult to achieve high quality crystal. In this work, we will describe a novel process to synthesize a device-grade GaN buffer layer by plasma immersion ion implantation (PIII) of nitrogen ions into a III-V semiconductor substrate followed by rapid thermal annealing. This thin surface layer of GaN can then be used for either direct device fabrication or as a lattice-matched template for further epitaxial growth of GaN. PIII offers the advantage of high efficiency and highly uniform beam density over a large area, which are particularly important for commercial and large wafer processing. PIII can be performed at low energy implantation thereby favoring the formation of thin layers. We will present our characterization results acquired by photoluminescence, Raman scattering, x-ray diffraction, Hall mobility and carrier concentration measurements.

SESSION K6: INTERDIFFUSION AND SEGREGATION

Chair: David E. Jesson
Wednesday Morning, April 26, 2000
Salon 1/2 (Marriott)

8:30 AM *K6.1

INTERACTIONS, INTERDIFFUSION AND SEGREGATION IN QUANTUM DOT ENSEMBLES. Rosa Leon, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA.

Statistically non-interacting quantum dot ensembles can be achieved by raising surface energies during growth [1]. This also produces large concentration variations in simultaneous growths of InGaAs quantum dots (QDs) by step edge nucleation control on vicinal GaAs [001]. These QD surface density variations radically affect their optical properties. Strong strain interactions between QDs in dense ensembles are seen to blue-shift emission energies, narrow inter-sub-level transition energies, shorten luminescence decay times for excited states, and increase inhomogeneous photoluminescence broadening [2]. These effects are compared to recent results obtained in QDs after InGaAs/GaAs interfacial compositional disordering [3]. Different

relaxation (capture and escape) mechanisms become predominant in isolated and interacting (high density) QDs, resulting in different temperature dependencies of PL energy shifts, intensities, inhomogeneous line-width broadening and rise times. Some of these observations are attributed to inhibited carrier capture and re-capture into the QDs. Low temperature carrier trapping at potential fluctuations in the wetting layer (WL) might be explained by Indium enrichment found in ternary InGaAs QDs [4] in terms of alloy variations in the Wetting Layer. Also of interest, is the finding that dot ensembles showing well-defined zero-dimensional properties are unstable against ripening. The impact of these findings on QD based device applications will be discussed. [1] R. Leon, C. Lobo, J. Zou, T. Romeo, and D.J.H. Cockayne, *Phys. Rev. Lett.* 81, 2486 (1998). [2] R. Leon, S. Marcinkevicius, X.Z. Liao, J. Zou, D.J.H. Cockayne, and S. Fafard, *Phys. Rev. B* 60, R8517 (1999) [3] R. Leon, S. Fafard, P.G. Piva, S. Ruvimov and Z. Liliental-Weber, *Phys. Rev. B* 58, R4262, (1998) [4] X.Z. Liao, J. Zou, D.J.H. Cockayne, R. Leon, and C. Lobo, *Phys. Rev. Lett.* 82, 5148 (1999).

9:00 AM *K6.2

NANOMETER-SCALE STUDIES OF INTERDIFFUSION AND SEGREGATION IN STACKED SELF-ASSEMBLED InAs/GaAs QUANTUM DOTS. R.S. Goldman, B. Lita, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI; J.D. Phillips, P.K. Bhattacharya, Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI.

Self-assembled quantum dots have been shown to develop during the epitaxial growth of highly-mismatched films in the Stranski-Krastanow growth mode. After the initial growth of a few monolayers wetting layer, island nucleation results in the formation of self-assembled quantum dots. Stacks of capped quantum dots can be used to form vertically ordered, three-dimensional dot lattices, which have novel electronic and optical properties. However, the mechanisms of dot uniformity and the limitations to the perfection of the dot lattices are not fully understood. Therefore, we have investigated the nanometer-scale structure of stacked self-assembled InAs/GaAs quantum dots using ultra-high vacuum cross-sectional scanning tunneling microscopy. We show that the stacked InAs/GaAs quantum dots have organized into a laterally uniform distribution of columns. As the number of dot layers in the stack is increased, the linear density of vertically organized columns increases, and the average spacing between them decreases. Surprisingly, the spacing between dot columns is constant throughout the thickness of a particular stack of dots, suggesting that bulk diffusion processes determine this length-scale. In addition, we observe lateral variations in the vertical positions of In atoms in both the dot stacks and wetting layers. In some regions, the wetting layer thickness is much less than the dot height. In other regions, the wetting layer thickness is greater than the dot height such that the dot is immersed in the wetting layer. We have performed In/Ga atom counting in order to achieve the first direct atom-level measurements of indium-gallium interdiffusion and indium segregation lengths. We will discuss the relative contributions of In surface segregation and post-growth In-Ga interdiffusion processes to the formation of both the dot stacks and the wetting layers. We will also discuss our progress towards the first direct atom-level measurements of indium-gallium interdiffusion coefficients.

9:30 AM K6.3

CATHODOLUMINESCENCE WAVELENGTH IMAGING OF MICRON-SCALE ENERGY VARIATIONS IN VERTICALLY SELF-ORGANIZED InAs/GaAs QUANTUM DOTS. C. Zhang, D.H. Rich, Q. Xie, P. Chen and A. Madhukar, Department of Materials Science and Engineering, University of Southern California, Los Angeles, CA.

We have examined the optical and structural properties of vertically self-organized (VSO) self-assembled quantum dot (SAQD) samples of InAs on GaAs(001). Single and multiple SAQD layers were grown by molecular beam epitaxy (MBE). We have found a spatial correlation between the energy and intensity fluctuations of luminescence from the broadened distribution of QDs. We employ a unique and powerful optical technique, termed cathodoluminescence wavelength imaging (CLWI), to enable a spatial mapping of the peak energy of the emission from the ensemble of QDs. CLWI is accomplished by acquiring a series of discrete monochromatic images, constructing a local spectrum at all 640 x 480 scan points within the image, and determining the wavelength at which there is a peak in the CL spectrum at each scan point. CLWI thus enables a spatial mapping of the effective band gap for interband transitions. We have observed a direct spatial correlation between a decrease in the energy of interband transitions with an increase in CL intensity on a scale of a few microns for a variety of VSO SAQD samples. The energy and intensity fluctuations are found to depend on the number of QD layers and interlayer spacing. Such fluctuations may reflect size/shape dependent variations in the carrier capture in the QDs, spatial variations in thermally induced reemission of carriers, and/or spatial

variations in the density of localized defects, which can act as nonradiative recombination sites. Temperature-dependent CL measurements are performed to assess which of the foregoing explanations is most plausible. On a scale of a few microns, CLWI reveals a tendency for InAs QDs to form constant energy clusters, within the typical cation migration length of In during MBE growth.

9:45 AM K6.4

InGaAs/GaAs QUANTUM DOT INTERDIFFUSION INDUCED BY CAP LAYER OVERGROWTH. J. Jasinski, Materials Science Division, Lawrence National Berkeley Laboratory, Berkeley, CA; A. Babinski, M. Czeczott, R. Bozek, Institute of Experimental Physics, Warsaw University, Warsaw, POLAND.

In a last few years self-organized quantum dots (QDs) attracted a lot of scientific interest mostly due to their optoelectronic applications in light emitting devices [1]. One of the most important problems in this field is a capability of tuning of QD emission wavelength. It has been proposed that a post-growth annealing of QDs layers can be applied in such a tuning [2]. It has been showed that such thermal treatment can lead to a large blueshift of the luminescence coming from QDs. This has been interpreted as a result of QD interdiffusion. In this study we demonstrate that a strong QD interdiffusion can also occur during growth of a cap layer covering layer of QDs. We examined self-organized InGaAs QDs grown on GaAs substrates and covered with two different types of cap layers grown at significantly different temperatures. The photoluminescence and transmission electron microscopy measurements were carried out in order to correlate optical and structural properties of QDs. A relatively large blueshift of QDs luminescence peak was observed in samples covered with cap layers grown at the higher temperature. However, no remarkable change in the QDs size distribution was observed. Our results indicate that a strong QD interdiffusion occurs in samples covered with cap layers grown at the higher temperature, which affects QDs photoluminescence emission. 1. N. Kirsteadter, N.N. Ledenstev, M. Grudmann, D. Bimberg, V.M. Ustinov, S.S. Ruvimov, M.V. Maximov, P.S. Kopev, Zh.I. Alferov, U. Richter, P. Werner, U. Gosele, and J. Heydenreich, *Electron. Lett.* 30, 1416 (1994). 2. R. Leon, Yong Kim, and C. Jagadish, M. Gal, J. Zou, and D. J. H. Cockayne, *Appl. Phys. Lett.* 69, 1888 (1996).

10:30 AM *K6.5

LATERAL AND VERTICAL ORDERING OF SELF-ASSEMBLED QUANTUM DOTS IN SEMICONDUCTOR SUPERLATTICES. Vaclav Holy, Masaryk University, Dept. of Solid State Physics, Brno, CZECH REPUBLIC; Gunther Springholz, Michael Pinczolitns and Gunther Bauer, J. Kepler University, Dept. of Semiconductor Physics, Linz, AUSTRIA.

Self-organization phenomena during epitaxial growth of crystalline superlattices have been of considerable interest due to their potential application in fabrication in nanostructures, since self-organized structures at a superlattice interface (self-assembled quantum wires and quantum dots) exhibit a useful optical activity. Quasi zero-dimensional quantum dots occur during the epitaxial growth in the Stranski-Krastanow growth mode. During the growth, the deformation energy of a growing strained layer is relaxed elastically and a disordered regular two-dimensional array of small islands is created. In a multilayer, the deformation field of a buried dot array propagates through the host crystal towards the free surface and modifies the chemical potential of the migrating adatoms. If the host crystal is elastically anisotropic, this mechanism leads to a nearly perfect three-dimensional ordering of the quantum dots resulting in a three-dimensional dot-crystal. The symmetry of the elastic properties of the host crystal determines the lattice type of the dot crystal. In particular, rhombohedral dot crystals have been observed in (111)-oriented IV-VI type superlattices (such as PbSe/PbEuTe), in more common II-VI (001)-oriented superlattices (CdZnSe/ZnSe) body-centered tetragonal dot crystals occur. In materials with weak elastic anisotropy (Ge/Si multilayers, among others) the dot positions are well correlated vertically whereas their lateral ordering is very weak. We have investigated the structure of the dot crystals by high-resolution x-ray diffraction, atomic force microscopy and cross-sectional transmission electron microscopy. The shape of individual quantum dots was determined by means of non-coplanar small angle x-ray scattering. We have also studied the kinetics of the dot nucleation using a simple Monte-Carlo numerical simulation. The experimental results agree well with numerical predictions and show the possibility to control the parameters of the dot crystal by changing the superlattice period.

11:00 AM K6.6

SPATIAL ORDERING OF STACKED QUANTUM DOTS. Choong-Seop Lee, Byungham Kahng, Albert-László Barabási, Dept of Physics, University of Notre Dame, Notre Dame, IN.

Recently, much effort has been devoted to the fabrication of stacked

quantum dots (QDs), potential candidates for applications in lasers and detectors. In this work, we investigate the growth conditions necessary to form an ordered QDs crystal by capping spatially ordered QDs and growing a new layer of dots on top of the capping layer. We performed Monte Carlo simulations and developed analytic arguments based on the stress energy function generated by an array of QDs to determine the optimal capping layer thickness, external flux and the temperature for QD crystal formation.

11:15 AM K6.7

A QUANTITATIVE MODEL OF SURFACE SEGREGATION IN III-V TERNARY COMPOUNDS. Sergey Yu Karpov, Vladimir F. Myrmin, Soft-Impact Ltd., St. Petersburg, RUSSIA; Yuri N. Makarov, Univ Erlangen-Nürnberg, Fluid Mechanics Dept, Erlangen, GERMANY.

We suggest a rate-equation kinetic model of surface segregation occurring during Molecular Beam Epitaxy of ternary III-V compounds. The basic assumption of the model is that the atoms accumulated in the adsorption layer on the surface of semiconductor are in partial equilibrium with the bulk of the crystal. Use of the assumption allows us to develop a quantitative model of surface segregation free from any fitting parameters (necessary kinetic rate constant are evaluated from the independent experimental data). The model was applied to a number of ternary III-V compounds which surface segregation is an important effect for (InGaAs, AlGaAs, etc.). The following aspects of this phenomenon were studied: dependence of segregation on temperature, growth rate, type and orientation of the substrate. The investigations show that the partial equilibrium between the adatoms and solid phase is the factor controlling both dynamics of temporal evolution and efficiency of surface segregation. That is why the elastic strain originated from the lattice constant mismatch between the substrate and epitaxial layer affects significantly the process of segregation. Under high temperatures desorption of group-III atoms from the growth surface becomes important and leads to lowering of the saturation level of solid phase composition. The theoretical predictions are compared with the experimental data available from literature. The comparison shows a good agreement between the theory and experiment. The model proposed can be easily extended to the case of other growth techniques.

11:30 AM K6.8

EFFECTS OF STRAIN-INDUCED SEGREGATION ON INTERFACIAL STRUCTURE AND STABILITY AND FILM SURFACE MORPHOLOGY IN LAYER-BY-LAYER SEMICONDUCTOR HETEROEPITAXY. Luis A. Zepeda-Ruiz, W. Henry Weinberg, and Dimitrios Maroudas, Department of Chemical Engineering, University of California, Santa Barbara, CA.

Grading the epitaxial film composition is a well established practice of reducing strain due to lattice mismatch in the heteroepitaxial growth of semiconductor thin films. Strain-induced segregation of the graded film constituents at the film/substrate interfaces and on interfacial defects can affect significantly the interfacial stability, the deformation field, and the electronic properties of the epitaxial film. In this presentation, we analyze such segregation effects on interfacial stability with respect to misfit dislocation formation, semicoherent interface structure, and film surface morphology in semiconductor heteroepitaxial systems with compositionally graded, layer-by-layer grown films. Our theoretical study combines a Canonical Metropolis Monte Carlo (CMMC) method with structural relaxation simulations based on a valence force field description of interatomic interactions. CMMC is used to model compositional relaxation and obtain species distributions as determined by the interfacial segregation driving forces, while local structural relaxation is performed according to a conjugate-gradient scheme for energy minimization. This computational methodology is applied to study strain-induced species segregation in the epitaxial growth of $\text{In}_x\text{Ga}_{1-x}\text{As}$ films on GaAs(111)A substrates; the prototypical film/substrate system at $x=1$ is characterized by very high compressive lattice-mismatch strain of about 7%. Special emphasis is placed on the analysis of segregation at interfacial misfit dislocations and faulted interfacial regions. Semicoherent interfacial structures and compositional distributions, as well as the resulting strain fields and film surface morphologies are analyzed in detail as a function of film thickness for given film composition. The computed surface morphologies are in good agreement with experimental measurements. Critical thicknesses for the coherent-to-semicoherent interface transition are calculated as a function of film composition. The simulation results are discussed within the framework of continuum elasticity and dislocation theory.

11:45 AM K6.9

EVOLUTION OF INTERFACE MORPHOLOGY AND SURFACE SEGREGATION IN $\text{ZnSnP}_2/\text{GaAs}$ SUPERLATTICES. B. Lita, M. Beck and R.S. Goldman, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI; G.A. Seryogin,

S.A. Nikishin, and H. Temkin, Department of Electrical Engineering, Texas Tech University, Lubbock, TX.

Due to its tetragonal unit cell and direct band gap in the near infrared, ZnSnP_2 is promising for a variety of applications including non-linear optical devices and solar cells. Furthermore, both ordered (chalcopyrite) and disordered (sphalerite) phases of ZnSnP_2 may be grown nearly lattice-matched to GaAs, providing a means for producing low misfit structures with a variety of band offsets. A remaining challenge in the preparation of $\text{ZnSnP}_2/\text{GaAs}$ heterostructures is the control of the vertical and lateral uniformity of the interface morphology and the alloy composition. Therefore, we have investigated the evolution of the interface structure and electronic properties in a set of gas-source molecular beam epitaxially grown $\text{ZnSnP}_2/\text{GaAs}$ superlattices using cross-sectional scanning tunneling microscopy and spectroscopy. These superlattices contain quantum wells of disordered ZnSnP_2 and barriers of GaAs. We observe lateral variations in the morphology of the ZnSnP_2 on GaAs interfaces. The amplitude of these undulations decreases gradually towards the top of the structure. Furthermore, we observe an asymmetry in interface abruptness, with the ZnSnP_2 on GaAs interfaces apparently much smoother than the GaAs on ZnSnP_2 interfaces. The increased roughness of the GaAs on ZnSnP_2 interface occurs simultaneously with surface segregation of cations. In addition, a higher density of cleavage steps is apparent in the proximity of the rougher GaAs on ZnSnP_2 interfaces, suggesting a higher residual strain at these interfaces. Hence, the mechanism for the interface asymmetry is likely to be strain-enhanced surface segregation of cations during the growth of GaAs on ZnSnP_2 . Finally, scanning tunneling spectroscopy measurements in the ZnSnP_2 regions reveal lateral variations in the effective band gaps of the layers. The interplay between growth surface undulations and lateral inhomogeneities in the ZnSnP_2 layers will be discussed.

SESSION K7: BAND STRUCTURE, ELECTRONIC PROPERTIES, AND DEVICES

Chair: Rachel S. Goldman
Wednesday Afternoon, April 26, 2000
Salon 1/2 (Marriott)

1:30 PM *K7.1

OPTOELECTRONIC DEVICE APPLICATIONS OF SELF-ORGANIZED $\text{In}(\text{Ga,Al})\text{As}/\text{Ga}(\text{Al})\text{As}$ QUANTUM DOTS. Pallab Bhattacharya, Sanjay Krishna, Jamie Phillips, Jasprit Singh, Hong-Tao Jiang, University of Michigan, Dept. of Electrical Engineering and Computer Science, Ann Arbor, MI.

Self-organized growth of strained semiconductor heterostructures has enabled the realization of ordered arrays of quantum dots which can be incorporated into the active region of electronic and optoelectronic devices. In the $\text{In}(\text{Ga,Al})\text{As}/\text{Ga}(\text{Al})\text{As}$ heterostructure system, the dots are 20 nm in lateral extent and 5-8 nm in height with a near pyramidal shape. The ground state transition energy can be varied from 0.7 to 1.9 μm with variation of dot composition, heterostructure and substrate (GaAs or InP). Photoluminescence linewidth (FWHM) as low as 19 meV have been measured for InAs/GaAs dots. The properties of multi-dot layer high performance edge-emitting lasers will be described. The bandwidth of these lasers are 5-7 GHz at 300K and ~ 30 GHz at 77K. From independent optical and electrical measurements we have established that an intrinsic limit to the bandwidth is set by electron relaxation times of 40ps and 10 ps at 300K and 4K, respectively. These times agree with theoretical calculations based on electron-hole scattering as a limiting mechanism. The differential gain in the lasers is as high as 10^{13} cm^2 . However, a limit to the highest achievable modulation bandwidth is imposed by the electron-hole scattering rate. The optoelectronic properties of the dots and the dynamics of carriers therein are extremely attractive for high-speed wavelength switching and the design of electro-optic modulators. We have measured the electro-optic coefficients in the quantum dots and the linear E-O coefficient is $r_l = 2.6 \times 10^{-11} \text{ m/V}$, comparable to that in LiNbO_3 . The large intersubband electron relaxation time in the quantum dot can also be used as an advantage for the design of intersubband lasers and detectors. We have fabricated and characterized intersubband detectors designed for vertical optical incidence. Detection at 5 μm has been recorded for intersubband detectors.

2:00 PM K7.2

MULTIPLY STACKED 1.3 MICRON $\text{InAs}/\text{InGaAs}$ QUANTUM DOT STRUCTURES GROWN BY MBE. Nikolai Maleev, Alexey Zhukov, Alexey Kovsh, Sergey Mikhlin, Victor Ustinov, Denis Bedarev, Igor Krestnikov, Yuri Musikhin, Vladimir Odnoblyudov, Andrey Tsatsulnikov, Piter Kopev, Zhores Alferov, A.F. Ioffe Physico-Technical Institute, St. Petersburg, RUSSIA; Nikolai Ledentsov, Dieter Bimberg, Technische Universität Berlin, Institut für Festkörperphysik, Berlin, GERMANY.

InGaAs quantum dot (QD) structures grown by MBE on GaAs are promising candidates for 1.3 micron light source applications [1]. To realize high-performance QD vertical-cavity surface-emitting lasers (VCSELs) and edge-emitting lasers, it is necessary to form highly uniform dense array of QDs. We have recently shown that the high surface density QD arrays which emit at 1.3 micron can be obtained by covering InAs QDs with a thin InGaAs layer [2]. The aim of this work is to study structural and photoluminescence (PL) properties of stacked InAs/InGaAs QD layers and to obtain the optimal growth conditions for 1.3 micron light source applications. The structures grown on (001) GaAs substrates consist of several layers of InAs/InGaAs QDs separated by GaAs spacers. The QDs were deposited at 485°C. For QD laser structures the spacer thickness is typically kept small (from 1.5 to 5 nm) which leads to the electronic coupling between the dots of adjacent layers. However, we have found that this approach does not work for the 1.3 micron InAs/InGaAs QD structures due to drastic decrease in PL intensity. We propose to use the relatively thick GaAs spacer layers (15-30 nm) consisting of two parts. First thin GaAs cap layer is grown at 480-500°C and the rest of the spacer is grown at 600°C. Such stacking of three QD planes results in a low threshold (70-85 A/cm²) long-wavelength (1.25-1.26 micron) lasing at room temperature (RT) with relatively high differential efficiency (>50%). Bright RT PL at 1.28-1.3 micron from vertical optical microcavities containing the 9 layers of InAs/InGaAs QDs is demonstrated.

[1] D.L. Huffaker, G. Park, Z. Zou, O.B. Shchekin, D.G. Deppe, Appl. Phys. Lett., 73, p. 2564 (1998)

[2] V.M. Ustinov, N.A. Maleev, A.E. Zhukov, A.R. Kovsh, A.Yu. Egorov, A.V. Lunev, B.V. Volovik, I.L. Krestnikov, Yu.G. Musikhin, N.A. Bert, P.S. Kop'ev, Zh.I. Alferov, N.N. Ledentsov and D. Bimberg, Appl. Phys. Lett., 74, p. 2815 (1999)

2:15 PM K7.3

STRONG PHOTON-EXCITON COUPLING IN THE NEAR-FIELD LUMINESCENCE OF SEMICONDUCTOR QUANTUM DOTS.
A.M. Mintairov, A.S. Vlasov, J.L. Merz, Notre Dame University, Dept of Electrical Engineering, IN; O.V. Kovalenkov, D.A. Vinokurov, Ioffe Physical-Technical Institute, St. Petersburg, RUSSIA.

We present low-temperature near-field scanning optical microscopy (NSOM) measurements of self-organized InP quantum dots (QD). We observed strong detuning of the emission energy of the QD structure by changing the tip-to-surface distance. The effect indicates formation of a near-field nano-cavity having extremely high photon-exciton mixing. The QDs have a base ~ 80 nm and density $\sim 10^9$ cm⁻², and are embedded in 0.35 μ m GaInP grown on GaAs by MOCVD. The near-field photoluminescence (PL) spectra were taken in collection-illumination mode at 10 K under 514.5 nm excitation of an Ar laser (power density 15 W/cm²). The experiments were done with a ~ 0.2 μ m fiber tip coated by 20 (type A tip) or 60 (type B) nm of Al. The near-field PL spectra of InP QDs measured with tips of type A consist of several discrete narrow lines and manifold bands in the range 1.7-1.95 eV, representing exciton emission from QD levels, wetting layer localized states, and the GaInP matrix. Typical spectra of single QD emission consists of a triplet manifold at ~ 1.72 eV having an energy splitting of 1-3 meV and a halfwidth of the high energy components < 200 μ eV. The position and relative intensity of the discrete emission lines and manifolds do not depend on tip-to-surface distance (Δz) for tips of type A. For tips of type B we observed a strong dependence of the near-field spectra on Δz . In this case the spectra are dominated by one manifold, the position of which changes linearly from 1.72 eV (721 nm) to 1.95 eV (636 nm) when Δz changes by only 100 nm. Such behavior implies the creation of a $3\lambda/2$ near-field nano-cavity formed by the GaInP-GaAs interface and the NSOM tip. The extremely strong linear detuning (85 nm) of the emission wavelength of the QD having discrete energy levels indicates on extremely strong coupling of photons and excitons in such a nanocavity.

2:30 PM K7.4

IMPROVED CARRIER TRANSPORT IN INTERMIXED GaAs/AlGaAs LASER STRUCTURE WITH MULTIQUANTUM WELL CLADDING. J.H. Teng, S.J. Chua, W. Liu, National Univ. of Singapore, Dept of Electrical Engineering, SINGAPORE; X.C. Wang, X.H. Zhang, G. Li, National Univ. of Singapore, Institute of Material Research and Engineering, SINGAPORE; D. Braddock, Ovation Semiconductor, Rochester, MN.

Quantum well (QW) intermixing has attracted considerable interest in the past decades due to its wide applicability in photonic integrated circuit and material characteristic study. The characteristics of the intermixed QWs as well as the methods to induce and suppress QW intermixing are widely studied. However, there is no report yet about the effects of the cladding layer structure on the QW intermixing by rapid thermal processing. In this paper, we report that after the QW intermixing process in GaAs/AlGaAs laser

structure with a multi-quantum well cladding layer, the carrier transport from the cladding layer to the quantum well region is much more efficient than that in the non-intermixed sample. Also the cladding layer and the quantum well showed a very different behavior in the photoluminescence (PL) spectra after QW intermixing. The multi-quantum well structure used in the cladding layer can improve the AlGaAs layer quality and improve both the electron and hole transport through the thick cladding layers and thus raise the overall efficiency of the laser. After rapid thermal annealing (RTA) with the silica capping at 850°C for 45s, the peak of the PL signal of the cladding layer showed a 93meV blueshift compared to 27meV for the quantum well. The full width at half maximum (FWHM) of the PL signal of the cladding layer reduced from 35.3meV to 19.9meV while that of the QW signal broadened from 6.9meV to 8.6meV. Temperature varied PL study showed a much greater intensity ratio between the QW and the cladding layer in the intermixed sample than that in original one. A reduced thickness fluctuation and better interface quality of the multi-quantum wells are responsible for the reduced carrier recombination in the cladding layer. The improvement in the carrier transport is beneficial to laser and other optoelectronic device performance.

3:15 PM *K7.5

EXCITONS RECOMBINATION ENGINEERING IN SELF-ASSEMBLED QUANTUM DOTS. P.M. Petroff, Materials Department, University of California, Santa Barbara, CA.

We demonstrate using band gap engineering in self assembled quantum dot structures that excitons can be stored for several seconds. The optically generated excitons are dissociated and stored as separated electron hole pairs into coupled quantum dot pairs. A bias voltage restores the excitons which recombine radiatively to provide a read out optical signal. The localization of the spatially separated electron hole pair in quantum dots is responsible for the ultra long storage times which are on the order of several seconds. The present limits of this optical storage medium are discussed.

3:45 PM K7.6

SCANNING TUNNELING SPECTROSCOPY INVESTIGATION OF THE STRAINED Si_{1-x}Ge_x BAND OFFSETS. Xiangdong Chen, Xiang-Dong Wang, Kou-Chen Liu, Dong-Won Kim and Sanjay Banerjee, Microelectronics Research Center, The University of Texas at Austin, Austin, TX.

The band offsets and band gap are the most important parameters that determine the electrical and optical behavior of a heterojunction. In situ scanning tunneling spectroscopy (STS) was employed to measure the valence band offsets of strained Si_{1-x}Ge_x-on-Si (100) for the first time. The valence band offsets of the strained Si_{0.77}Ge_{0.23} and Si_{0.59}Ge_{0.41} on Si(100) are found to be 0.21eV and 0.36eV, respectively. The results are in good agreement with theory and with results from other experimental methods. Due to band bending and surface states, it is difficult to determine the conduction band edge at the interface of the Si_{1-x}Ge_x/Si exactly but we find that the conduction band offset is much smaller than the valence band offset.

4:00 PM K7.7

INTERFACE CONTROL AND BAND OFFSET AT THE GaInP ON GaAs HETEROJUNCTION. Cheng Cai, Marshall I. Nathan, Department of Electrical and Computer Engineering, University of Minnesota, Minneapolis, MN.

We measured current versus voltage (*I-V*) and capacitance versus voltage (*C-V*) characteristics of lattice matched GaInP/GaAs heterojunctions with Schottky barriers grown by gas source molecular beam epitaxy (GSMBE). The difference of Schottky barrier heights measured by *I-V* (Φ_{IV}) and *C-V* (Φ_{CV}) was found to be related to the band offset and interface charge between GaInP and GaAs. The band offset and interface charge were determined by varying the thickness of the undoped GaInP layer. The existence of interface charge is considered as the consequence of compositional intermixing and localized strain at phosphide/arsenide interface. A new growth switching procedure from GaAs layer to GaInP was applied to improve the interface quality. We found that lower interface charge density between GaInP was achieved by exposing GaAs surface to Ga solid source instead of thermally cracked AsH₃ or PH₃ before starting GaInP layer growth. The exposing time was from 24s up to 64s. The interface charge density was reduced from 8.7×10^{11} cm⁻² to less than 4.7×10^{11} cm⁻². The band offset was shown to be strongly dependent on the interface condition. This fact is an indication that a large dispersion in the reported values of the band offset of GaInP/GaAs is related to the lack of precise control of the interface.

4:15 PM K7.8

BANDGAP TUNING BY A Ge LAYER IN QUANTUM WELL INTERMIXING. J.H. Teng, S.J. Chua, National Univ of Singapore, Dept of Electrical Engineering, Singapore, SINGAPORE; G. Li,

National Univ of Singapore, Institute of Material Research and Engineering, Singapore, SINGAPORE; A. Saher Helmeý, J.H. Marsh, Univ of Glasgow, Dept of Electronics and Electrical Engineering, UNITED KINGDOM.

Impurity-free vacancy enhanced quantum well intermixing is an easy and effective way for the fabrication of photonic integrated circuit. One key technology is the selective modification of the band gap energy of quantum wells across a wafer. Usually SiO₂ film is used to induce the Ga out-diffusion so as to enhance the quantum well intermixing; SrF₂ or Si₃N₄ is used to inhibit the quantum well intermixing. In this paper, we report that a novel and simple technique for controlling the band gap shift in AlGaAs/GaAs and InGaAs/GaAs quantum well (QW) structures. It involves evaporation of a thin Ge layer and then covering the sample with a spin-on silica film followed by rapid thermal annealing. The quantum well intermixing was suppressed in the presence of this Ge layer buried between the sample surface and the SiO₂. The interdiffusion rate was reduced by more than one order of magnitude compared to that without the Ge interlayer. The blue shift of the band gap can be controlled by varying the thickness of the buried Ge layer. Differential band gap shift over 100meV can be achieved with a 50nm Ge interlayer for both the AlGaAs/GaAs and InGaAs/GaAs QW structures. The optical quality of the material was not deteriorate by the Ge covering compared to SiO₂ covering in view of the photoluminescence intensity and spectral linewidth. The possible mechanism for the suppress of quantum well intermixing by the Ge interlayer is proposed. Using appropriate mask, this technique has the potential to tune the band gap shift in different areas across a single wafer.

4:30 PM **K7.9**

A PHOTOREFLECTANCE STUDY OF N-TYPE GaSb AT E₀ and E₀+Δ₀ TRANSITIONS. S. Iyer, S. Mulugeta, B. Gong and Yusuf Farah, Department of Electrical Engineering, North Carolina A&T State University, Greensboro, NC; K.K. Bajaj and G. Coli, Department of Physics, Emory University, Atlanta, GA.

In this work, the use of photoreflectance (PR) technique has been demonstrated for the determination of carrier concentration in n-doped GaSb. This is particularly attractive in this material system, where due to the absence of semi-insulating substrates, the determination of the carrier concentration has posed a major problem in homo-epitaxially grown epilayers. In this study, PR response of bulk and epitaxially grown n-doped GaSb samples at the fundamental gap E₀ and at the higher energy transition E₀+Δ₀ from 4 to 250K has been investigated. The PR spectra are described using the third derivative of the Lorentzian functional form of the dielectric function. Using lineshape analysis of the PR spectra, the temperature dependence of the E₀ and E₀+Δ₀ transition energies has been obtained. The values of the E₀ and E₀+Δ₀ transition energies in a bulk grown sample with an electron concentration of about 1.6 x 10¹⁷/cm³ were found to be 0.830 and 1.583 eV at 4K, respectively. A systematic study has been carried out to correlate the shifts in the E₀ and E₀+Δ₀ transition energies at 4K with carrier concentrations in the epilayers. Including many-body effects such as band filling and band-gap renormalization in the analysis of the PR spectra, provides a good agreement between the computed values of the carrier concentration with those determined from Hall measurements. To the best of our knowledge this is the first report on the photoreflectance study in n-GaSb.

SESSION K8: MORPHOLOGY AND MICROSTRUCTURE

Chairs: Joanna Mirecki Millunchick and Peter W. Voorhees
Thursday Morning, April 27, 2000
Salon 1/2 (Marriott)

8:30 AM *K8.1

IN-SITU UHV MICROSCOPY OBSERVATIONS OF THIN FILM GROWTH. R.M. Tromp, IBM T.J. Watson Research Center, Yorktown Heights, NY.

In-situ UHV microscopy (LEEM, UHV-TEM) of SiGe/Si growth has been used to study fundamental processes in thin film growth: dislocation formation and interaction at low misfit, instability-driven surface roughening at intermediate misfit, and islanding at large misfit. I will present a comprehensive overview of these results. In addition I will briefly discuss recent observations on the growth of organic semiconductor films on a variety of substrates.

9:00 AM **K8.2**

CHARACTERIZING THE SURFACE COMPOSITION AND THE MORPHOLOGY OF SiGe FILMS IN MBE GROWN DEVICES.

Glenn G. Jernigan and Phillip E. Thompson, Naval Research Laboratory, Washington, DC.

We have developed a unique system for the investigation of the composition, via x-ray photoelectron spectroscopy (XPS), and of the morphology, via scanning tunneling microscopy (STM), of SiGe/Si heterostructures. The XPS and STM instruments are connected in vacuo to a VG-V80 molecular beam epitaxy (MBE) system designed for production of 3 inch SiGe device wafers. We will present an XPS and STM study of Si_{1-x}Gex (x=0.05-0.4) films grown on Si (100) between 350-800 C and at 1-100 nm thickness. XPS measurements show that Ge segregation occurs at the start of alloy growth producing a transition region between SiGe and Si. With increasing growth temperatures, intermixing occurs into the Si substrate and increases the thickness of the transition region. The intermixing does not change the total amount of Ge segregation found after the transition region. The amount of Ge segregation is related to the composition of the alloy. For SiGe alloys studied more than a monolayer of Ge segregation is found on the top surface. STM measurements show that the morphology of the SiGe films vary with alloy composition and temperature. At a fixed composition, the SiGe morphology can evolve from planar to rippled and finally to a 3D island morphology (quantum dots and huts) with increasing temperature while still having the same amount of segregated surface Ge. The presence of segregated Ge lowers the barrier to making additional surface area to relieve the SiGe film stress. We will present a physical model for the Ge segregation and surface morphology which evolves during MBE and discuss its relevance to device fabrication.

9:15 AM **K8.3**

COMPOSITION MODULATIONS IN TENSILE STRAINED InGaAs FILMS GROWN ON InP SUBSTRATES. X. Wu and G.C. Weatherly, Dept. of Materials Science and Engineering, McMaster University, Hamilton, CANADA.

The correlation between compositional modulations and surface morphology has been studied by TEM and AFM techniques for a series of InGaAs films grown by molecular beam epitaxy on (100) InP substrates. At low values of strain (+0.6%) the InGaAs films develop a coarse faceted structure on (411) and (4 $\bar{1}$ 1) planes after ~100 nm of film growth. Composition modulations (scaling with the size of the facets) are observed in films 0.1 to 1 μm thick, but in thicker films (>1μm) the faceted structure disappears while the scale of the compositional modulations decays to that found in unstrained films. On the other hand +2% strained InGaAs films show pronounced faceting with no evidence for compositional modulations in thicker films. The results are discussed in terms of the role of stress in promoting faceting and the position of the chemical spinodal in the ternary In-Ga-As system.

9:30 AM **K8.4**

THE GROWTH OF HIGH QUALITY In_{0.25}Ga_{0.75}AS EPILAYERS ON GaAs SUBSTRATES. G.W. Pickrell, K.L. Chang, J.H. Eppele, K.Y. Cheng and K.C. Hsieh, Department of Electrical and Computer Engineering and Microelectronics Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL.

The lack of high-quality substrates with different lattice constants has limited the alloys that can be grown for device use. Important devices such as 1.3 μm vertical cavity surface emitting lasers (VCSELs) as well as high speed transport devices would benefit from substrates with lattice constants between GaAs and InP. Pseudomorphic growth on these substrates has allowed the growth of thin In_xGa_{1-x}As layers, but indium mole fractions of 25-30% are still unreachable in thick layers. These thin layers work well in transport devices but optical devices require much thicker structures. Recently, metamorphic growth, which utilizes thick buffer layers, has been used to grow high electron mobility transistors (HEMTs) with higher indium compositions, but optical devices have yet to be demonstrated with this technique. Early work¹ in metamorphic growth of In_xGa_{1-x}As on GaAs showed that threading dislocations tended to move into the GaAs substrate for indium compositions of 18% or lower. Indium compositions of 18% to 28% showed threading dislocations moving into the GaAs substrate as well as the In_xGa_{1-x}As epilayer. In this study, we explored the growth conditions and the corresponding dislocation densities for In_{0.25}Ga_{0.75}As in an effort to achieve a high quality, relaxed epilayer. Effects of factors such as growth temperature, growth rate, arsenic overpressure and thickness were determined using transmission electron microscopy. Low growth temperatures in the range of 250°C to 450°C were investigated. For the first time, our results clearly show the gradual increase of misfit dislocations with increasing layer thickness. Due to the low growth temperatures used, the critical thicknesses seen in these samples were much larger than those predicted by conventional theory². By adjusting the substrate temperature, growth rate and arsenic overpressure, high quality epilayers with defect densities of less than 10⁶ cm⁻³ have been grown.

¹V. Krishnamoorthy, P. Ribas and R.M. Park, Appl. Phys. Lett. 58,

2000, (1991). ²J.W. Matthews and A.E. Blakeslee, J. Crystal Growth, 27, 118, (1974).

9:45 AM **K8.5**

COOPERATIVE NUCLEATION LEADING TO RIPPLE FORMATION IN InGaAs/GaAs FILMS. Nehal Chokshi and Joanna Mirecki Millunchick Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI.

In_{0.27}Ga_{0.73}As epilayers were grown on GaAs (001) substrates (1.87% misfit strain) by Molecular Beam Epitaxy to investigate the 2D to 3D transition as a function of thickness, *t*. The morphological evolution of the In_{0.27}Ga_{0.73}As epilayer proceeds through 3 distinct regimes as observed by Reflection High Energy Electron Diffraction and Atomic Force Microscopy. For the first five deposited monolayers the growth commenced in a layer-by-layer growth mode (regime 1). Indium induced smoothing was also observed in this regime. The second regime, $5 < t < 20$ MLs, exhibits the cooperative nucleation of islands and pits. That is, islands and pits nucleated in a sequential fashion. The third regime of growth, $t > 20$ MLs, involves the formation of ripples resulting from the coalescence of islands and pits. This rippled morphology is generally aligned along the $[1\bar{1}0]$ direction, but also exhibits a secondary alignment roughly along the $\langle 310 \rangle$ type directions. This implies that the islands are bound by $\{13n\}$ faces. These results indicate that ripple formation is a direct result of the cooperative nucleation and coalescence of islands and pits as opposed to the growth of a perturbation instability.

10:30 AM ***K8.6**

KINETICALLY-DRIVEN GROWTH INSTABILITY IN STRESSED SOLIDS. Michael J. Aziz and William Barvosa-Carter, Harvard University, Division of Engineering and Applied Sciences, Cambridge, MA; L.J. Gray and T. Kaplan, Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN.

We report a stress-induced kinetically-driven morphological instability of general applicability to driven systems. The effect of stress on the interfacial mobility couples to stress variations along a perturbed planar growth front, resulting in amplification of the perturbation. Experimentally we studied a model system in which stress is applied externally to a chemically pure substance, permitting us to isolate the effect of strain from any possible effects of composition. Measurements were made of the amplification rate with and without stress during solid phase epitaxial growth at a Si(001) interface with submicron-sized corrugations introduced lithographically. A quantitative comparison of theory and experiment, with no adjustable parameters, indicates that the new mechanism is required to account for the observed growth of the corrugation amplitude. This kinetically-driven mechanism operates in conjunction with the known diffusional instability and elastic strain energy-driven instability mechanisms in determining morphological evolution in nonequilibrium systems.

11:00 AM ***K8.7**

A THEORETICAL STUDY OF TWO DIFFERENT SYSTEMS WITH SURFACE STRAIN MODULATION (FROM AN ATOMISTIC POINT OF VIEW): ROUGHNESS ASSISTED ALLOY DEMIXING AT A GROWTH FRONT AND SYSTEMS WITH BURIED DISLOCATION NETWORK. C. Priester, IEMN, Dept ISEN, Villeneuve d'Ascq, FRANCE.

We will concentrate on two points: First, how the possibility of a better strain relaxation introduced by the surface roughness can modify alloy demixing is investigated. For this, the growth process on a rough surface is simulated by making use of a step by step model. The ternary alloy is described from an atomistic point of view and surface tension is taken into account. The balance between mixing enthalpy, strains, and the difference of surface tension between the two binaries which form the ternary alloy is discussed. How the alloy demixing is either enhanced or lowered by compositional effects is also considered. Secondly, one considers the so-called compliant substrates that result from the bonding of the thin layer on a substrate, the bonding imposing a twist or tilt angle. The two limiting cases of large and small angles are investigated, in order to consider two opposite potential uses of this buried grain-boundary, when a strained layer is overgrown: either creating a weak interface that could easily allow the motion of misfit dislocations strictly located at this buried interface, or creating a strain pattern at the surface, strong enough for ordering self-nucleated 3D islands.

11:30 AM **K8.8**

COMPOSITIONAL INSTABILITIES IN Sn_xGe_{1-x} AND Sn_xSi_{1-x} ALLOYS GROWN BY MOLECULAR BEAM EPITAXY. Regina Ragan, Kyu S. Min, Harry A. Atwater, Thomas J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, CA.

Sn_xGe_{1-x} and Sn_xSi_{1-x} alloys are interesting material systems since

they are the only class of group IV material that exhibit a direct energy bandgap. An indirect to direct energy transition has been demonstrated for compositionally homogeneous Sn_xGe_{1-x} alloys with $X > 0.11^1$. However, the incorporation of Sn in a Si or 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, unfavorable for homogeneous alloy formation, can be utilized in the formation of Sn quantum dots and possibly quantum wires. During epitaxial growth of Sn_xGe_{1-x} alloys on Ge(001) at $T = 150^\circ\text{C}$ 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 μm . For the Sn_xGe_{1-x} alloy with $x = 0.03$, the lateral composition modulation is extremely regular, having a period of 40-50 nm. The phase separation is not related to dislocation formation. 100 nm thick Sn_xGe_{1-x} alloys do not exhibit any variation in composition implying that the compositional instability evolves during growth of thicker films, e.g. 1 μm . Optical and structural characterization of 1 μm phase separated Sn_xGe_{1-x} alloys will be compared to that of homogeneous alloys. In the Sn_xSi_{1-x} system, coherently strained α -Sn dots within a defect-free Si(001) crystal are fabricated by phase separation of an epitaxially stabilized thin Sn_xSi_{1-x} diamond cubic solid solution embedded in Si(001). Phase separation of the thin alloy film and subsequent evolution occurs via growth and coarsening of regularly-shaped α -Sn quantum dots that appear as 4-6 diameter tetrakaidecahedra with facets oriented along elastically soft $\langle 100 \rangle$ directions. Attenuated total reflectance infrared absorption measurements indicate an absorption feature due to the α -Sn quantum dot array with onset near 0.3 eV and absorption strength of $8 \times 10^3 \text{ cm}^{-1}$. Further optical characterization will be discussed. ¹G. He and H.A. Atwater, Phys. Rev. Lett. 79, 1937 (1997)

11:45 AM **K8.9**

EVOLUTION OF MICROSTRUCTURE IN STRAIN-RELAXED InGaP FILMS GROWN BY MOVPE. Andrew Y. Kim, Lisa M. McGill, Eugene A. Fitzgerald, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA.

Graded buffers used to integrate semiconductors of dissimilar lattice constant feature dramatically changing materials properties and significant strain in potentially phase-separable alloys, yet the study of microstructural evolution in these systems has been limited primarily to dislocation structure. We recently discovered that previously unreported defects dominate the evolution of microstructure in MOVPE-grown graded buffers of InGaP on GaP [$\nabla_x(\text{In}_x\text{Ga}_{1-x})\text{P}/\text{GaP}$] when graded to compositions of $x > 0.2$. The new defects, which we call branch defects, are roughly 110 planar features orthogonal to the (001) growth surface that possess sharp local strain fields, thus can strongly affect dislocation dynamics in graded buffers. Branch defect morphology is dominated by growth temperature, where their density decreases and their strength increases with increasing temperature. Branch defects appear linked with the formation and coalescence of growth step terraces, which also decrease in density and increase in height with increasing temperature in $\nabla_x(\text{In}_x\text{Ga}_{1-x})\text{P}/\text{GaP}$. Structurally, branch defects occur orthogonal to terraces and create cusps in the terraces where they intersect. Surprisingly, strong branch defects appear as gentle surface valleys, while weak ones cause sharp surface features. At low growth temperatures, branch defects resemble lateral composition modulation observed in similar systems, although preliminary scanning transmission electron microscopy shows no measurable phase separation. While the nature of branch defects is still under study, process optimization for branch defect control has so far reduced dislocation density three orders of magnitude in $\nabla_x(\text{In}_x\text{Ga}_{1-x})\text{P}/\text{GaP}$. Even when branch defects are too weak to block dislocations, subtle changes in their morphology affect intensity and spectral width in light-emitting diodes (LEDs), so further optimization is under way. Evidence of branch defects has also been seen in lattice-matched systems and in other alloys, including InGaAs and GaAsSb. We will present an analysis of materials and LED characterization relating to branch defects and our current understanding of their evolution.

SESSION K9: NITRIDES

Chairs: Eric D. Jones and Normand A. Modine
Thursday Afternoon, April 27, 2000
Salon 1/2 (Marriott)

1:30 PM **K9.1**

COMPOSITIONAL EVOLUTION AND STRUCTURAL CHANGES DURING ANNEAL OF GROUP III-NITRIDE-ARSENIDE ALLOYS. S.G. Spruytte, C.W. Coldren, A.F. Marshall, J.S. Harris, Solid State and Photonics Laboratory, Stanford University, CA; M.C. Larson, Lawrence Livermore National Laboratory, CA.

InGaAs is a promising material system for active regions of 1.3 μm and 1.55 μm opto-electronic devices grown on GaAs substrates. Adding Nitrogen reduces the bandgap and relieves some of the misfit strain allowing a higher Indium concentration. However, due to the divergent properties of nitride and arsenide materials, the N mole fraction that can be incorporated into solid solution is limited. Precipitation is avoided by lowering the growth temperature. Surface reconstruction not only raises the practical achievable solubility limits but might also result in higher concentration of interstitials above the sites under tension. Growth of group III-Nitride-Arsenide materials was performed by elemental source molecular beam epitaxy employing a nitrogen r.f. plasma cell. Edge emitting lasers and VCSELs with InGaAsN active regions were fabricated and had emission wavelengths in the range of 1.2-1.25 μm . To decrease non-radiative recombination due to point defects, the InGaAs material must be annealed. Annealing not only improves the luminescence efficiency, it also results in a blue-shift of the emission spectrum. The understanding of the mechanisms responsible for this shift is critical for the optimization of the thermal cycle the active region undergoes during growth of layers above it. Samples annealed for different times and at different temperatures were characterized by photoluminescence, SIMS, and TEM. Compositional changes due to diffusion of nitrogen and point defect enhanced diffusion of Indium are most likely responsible for the blue shift.

1:45 PM K9.2

EFFECTS OF NITROGEN ON THE BAND STRUCTURE OF GaNP ALLOYS. H.P. Xin and C.W. Tu, Dept of Electrical and Computer Engineering, University of California, San Diego, La Jolla, CA; Yong Zhang and A. Mascarenhas, National Renewable Energy Laboratory, Golden, CO.

There is an increasing interest in the growth of III-N-V compounds because of the possibility of lattice-matching to Si, such as GaN_{0.02}P_{0.98}. Bellaiche et al. predicted a transition from indirect to direct bandgap at a very low N concentration for GaNP alloys. The dislocation density may also be reduced due to lattice-matching to Si, leading to an improvement of the material quality and the possibility of integrating GaNP with Si electronics technology. We report that incorporation of N in GaN_xP_{1-x} alloys ($x \geq 0.43\%$) leads to a direct bandgap behavior of GaNP. The GaNP bulk and GaNP/GaP multiple quantum wells (MQW) samples were grown on (100) GaP substrates by gas-source MBE with a RF nitrogen radical beam source. The samples were characterized by X-ray rocking curves and photoluminescence (PL) measurements. For N concentration lower than 0.43%, a series of sharp emission lines from the various N pair centers were observed for GaNP bulk layers. With increasing N concentration ($\geq 0.43\%$), strong PL emission from GaNP bulk layers was observed at room temperature for the first time, suggesting a direct bandgap behavior of GaNP alloy. The PL peak red-shifts with higher N concentration, but the intensity remains in the same scale. Due to a strong interaction between the narrow band of localized N states and the GaP conduction band matrix, the N-related resonant band moves downward and forms a relatively flat conduction band minimum. Consequently, GaN_xP_{1-x} ($x \geq 0.43\%$) alloys behave like a direct bandgap material. With increasing N concentration, this flat conduction band further shifts down due to a stronger repulsion interaction between these two bands, which accounts for the N-induced reduction of the fundamental band-gap energy. By using an infinite barrier height model and measuring PL emission energy as a function of well thickness, a large conduction-band effective mass $m_c^* \approx 0.9$ is obtained for GaN_{0.025}P_{0.975} alloy, confirming the formation of a flat conduction band minimum for GaNP alloy.

2:00 PM K9.3

BALLISTIC ELECTRON EMISSION SPECTROSCOPY IN Au/GaAs_{1-x}N_x. Michael Kozhevnikov, Venkatesh Narayanamurti, Chavva Reddy, Harvard Univ, Div. of Engineering and Applied Sciences, Gordon McKay Laboratory, Cambridge, MA; Huoping Xin, Charles Tu, Univ of California at San Diego, Dept of Electrical and Computer Engineering, La Jolla, CA.

After its creation in 1992, a direct bandgap dilute GaAs_{1-x}N_x has attracted considerable attention due to its significant bandgap reduction (more than 400 meV at $x \sim 0.04$) which is indicative of giant bandgap bowing. Nitrogen incorporation also results in a number of unusual optical and electronic properties (e.g. strongly non-linear pressure dependence of the bandgap, anomalous electron effective mass increase and observation of new interband optical transitions). Despite the obvious progress in the experimental and theoretical study of GaAsN anomalies, the underlying physical mechanisms are still under question. Our experimental approach in studying the dilute GaAsN band structure is to employ Ballistic Electron Emission Microscopy (BEEM), which is a powerful low-energy tool for nondestructive local characterization of the spatial and electronic properties of semiconductor heterostructures. In BEEM, the energy and angular distributions of hot electrons are controlled

independently on the semiconductor structure by changing the tip potential. Spectra obtained in the second derivative (SD) BEEM can be related to the band structure of the material under study. Here, we report on BEEM and SD-BEEM spectroscopic study of Au/GaAsN heterostructures for probing the effect of nitrogen incorporation on the band structure at low nitrogen concentrations (up to 2.1%). The SD-BEEM spectra show two main peaks, which we associate with the contribution of the Γ -like and L-like bands of GaAsN. As the nitrogen concentration increases, the energetic separation between these peaks increases as well, with a relative decrease of the L-like band contribution to the BEEM current. Another prominent effect of the nitrogen incorporation is a strong decrease of the Au/GaAsN Schottky barrier, from ~ 0.92 eV at $x=0$ down to ~ 0.55 eV at $x=0.021$. These measurements shed new light on the effect of nitrogen in determining the band structure of the material.

2:15 PM K9.4

GROWTH OF GaInNAs BY PLASMA ASSISTED MOLECULAR BEAM EPITAXY. David W. Gotthold, Sridhar Govindaraju, Archie L. Holmes, Jr., Ben G. Streetman, Texas Materials Institute and Microelectronics Research Center, The University of Texas at Austin, Austin, TX.

The quaternary GaInNAs has attracted a great deal of interest recently for optoelectronic device applications at long wavelengths, especially 1.3 μm . This material has the potential to reach 1.55 μm for long-haul fiber optic communications by the addition of more indium and nitrogen into GaAs. However, this causes structural and optical properties to degrade. The cause of this degradation is unclear: it may be fundamental to the material or may be due to unoptimized growth conditions. In this work we systematically explore the parameter space for the growth of GaInNAs using plasma-assisted MBE and inert gas dilution. Inert gas dilution allows additional control of the production of active nitrogen; thus we can independently adjust RF power, gas flow rate, and nitrogen generation, which is used to study the effects of the plasma on the growth surface. In addition to examining the effects of plasma operating conditions, we will also explore the effects of other growth parameters (arsenic to nitrogen ratio and growth temperature) on the resultant structural and optical properties. These properties will be explored by photoluminescence, SIMS, and x-ray diffraction with the goal of understanding the effect of how nitrogen incorporation affects the resultant material property.

3:00 PM K9.5

LOCAL ORDERING IN GaN-RICH TERNARY GaNP ALLOYS. R.K. Soni, P.S. Dabal, R.S. Katiyar, Dept of Physics, University of Puerto Rico, San Juan, PR; H. Asahi, S. Gonda, Institute of Scientific and Industrial Research, Osaka University, Osaka, JAPAN.

Anomalous large band bowing parameter and a possibility of strong ordering effects has attracted considerable theoretical interest in GaN(As,P) ternary alloys. Presence of a large miscibility gap in GaNP ternary alloy due to the differences in the lattice constants and lattice structure, poses a major problem in the growth of high quality epitaxial layers. Using micro-Raman scattering we have studied atomic distribution and the ordering effects in GaN-rich side of the GaNP layers on (0001) sapphire substrates grown by electron cyclotron resonance molecular beam epitaxy (ECR-MBE). Low temperature photoluminescence indicates a red shift and significantly large band bowing parameter. Raman spectrum from layers grown at higher temperatures ($\geq 700^\circ\text{C}$) shows coexistence of GaP-rich region with cubic symmetry and GaN-rich region with hexagonal symmetry. Sharp TO and LO phonon lines indicative of (111) ordering in the GaP region are observed. Increasing phosphorous ($P > 1.5\%$) in the GaNP alloy leads to phase separation that is reflected in the suppression of GaN-like Raman modes. The phase-separated region shows an additional Raman line at 384 cm^{-1} between the TO and LO phonon of GaP due to strongly confined LO phonon in ordered (111) (GaP)_n(GaN)_m nanometer size clusters. Decreasing growth temperature increases the phosphorous concentration in the GaNP layer and disorder activated acoustic modes appear in the Raman spectrum as a result of symmetry break down. When phosphorous concentration reaches 8.2% in the layer grown at 570°C , Raman spectrum shows broad amorphous like bands indicative of short-range ordering. From polarized Raman scattering we have determined changes in the selection rules for TO and LO phonons in the GaNP alloy. This work is supported by NASA-NCC8-113 grant.

3:15 PM K9.6

CHARACTERIZATION OF STRAIN, TEXTURE AND INTER-FACE ROUGHNESS IN NITRIDE FILMS. M.R. Sardela, Jr., Materials Research Laboratory, University of Illinois, Urbana, IL; A. Li-Fatou, Charles Evans & Associates, Redwood City, CA; M. Jenkins and M.-A. Hasan, Dept of Electrical and Computer Engineering, University of North Carolina, Charlotte, NC.

Nitride-based materials have recently gained greater attention due to

the multitude of their utilization in microelectronics, optoelectronics, and hard-coating industries. TiN, for instance, is used as a diffusion barrier in Si microelectronics and as a hard coating in the tools industry. At the same time, developments in group-III nitrides have led to commercialization of laser diodes operating in the full range of visible light. However, device performance is directly tied to the material quality. Understanding their microstructural properties as a function of growth and post-growth treatment processes and developing precision non-destructive testing methods are crucial. In this study we investigate processes of strain relaxation, texture and interface roughness in thin films of TiN and AlN grown on Si substrates. Modern x-ray analytical methods using two-dimensional mapping of diffraction (XRD) and reflectivity (XRR) are employed, and the results are correlated with the findings from atomic force microscopy, transmission electron microscopy and secondary ion mass spectrometry. Ultra-thin TiN films, with thickness down to 8 nm, grown by chemical vapor deposition under conventional industrial environment were investigated. Ultra-thin materials, currently demanded by the constant trends of device miniaturization, are typically a problem for conventional XRD techniques due to the small volume available for scattering. The use of XRR in combination with simulations allowed the quantification of thickness and composition uniformity, and interface roughness. Also, a comparison of roughening prior and after plasma treatment is given. XRR mapping of diffuse scattering allowed the investigation of roughness correlation. Reciprocal lattice mapping of single-crystalline AlN films grown on Si by molecular beam epitaxy under various conditions, allowed for a separation between strain and defects contributions to the scattering distribution. Independent determination of in-plane and normal-to-the-surface strain components in the films was possible. The relationship between lattice mismatch, strain relaxation, substrate miscut and various growth parameters, is discussed.

3:30 PM **K9.7**

EFFECTS OF THE DISLOCATION DENSITY AND SURFACE ENERGY ON PHASE DIAGRAMS OF THE S-K GROWTH MODE FOR THE GaInN/GaN AND GaPSb/GaP SYSTEMS.

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The growth of thin films has been categorized into three types namely the Frank-van der Merwe (FM) mode, the Stranski-Krastanov (SK) mode, and the Volmer-Weber (VW) mode. These growth modes are deduced from considerations of the energy balance between the strain, surface, and interface energies. The SK mode has received much interest due to fabrication of self-assembling quantum dots. In order to identify the kind of system in which quantum dots can be easily formed, we have determined the thickness-composition phase diagrams of the growth modes for seven III-V ternary systems [1]. The phase diagrams are expressed as functions of the thickness and composition of the film and cluster. However, the effect of the dislocation density on the strain and interfacial energies, and the effect of the reconstruction of dangling bonds on the surface energy have not been considered for the calculation of these phase diagrams. In this work, the strain, surface, and interfacial energies were calculated for the three types of growth mode of the GaInN/GaN and GaPSb/GaP systems by considering the effects of the dislocation density and reconstruction of dangling bonds. The calculation method is essentially the same as the previously reported one [1]. We determined the phase diagrams of the growth modes for the GaInN/GaN and GaPSb/GaP systems. In the GaInN/GaN system, the VW mode appears in the most region of the phase diagram. The region of the VW mode becomes smaller as the dislocation density increases. In the GaPSb/GaP system, the SK and VW modes appear and the region of these modes becomes larger as the reconstruction ratio increases. From these phase diagrams, it is made clear that the region of the SK and VW modes is strongly affected by the dislocation density (or the strain energy) and the surface energy-change. [1] K. Nakajima, Jpn. J. Appl. Phys. 38, 1875-1883 (1999).

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STRUCTURAL INVESTIGATIONS OF (GaIn)(NAs) MULTI-QUANTUM-WELLS BY HIGH RESOLUTION TEM. Kerstin Volz,

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Mixed III-V nitride semiconductor alloys have a theoretically predicted large bandgap bowing, which would allow to realize 1.3 to 1.55 μm wavelength emission based on GaAs substrates. In this study, the novel quaternary material (GaIn)(NAs) was grown at low substrate temperatures by MOVPE using for group V precursors UDMHy and TBAs, and for group III precursors TEGa and TMIIn. Systems of up to 10 quantum-wells are formed compressively strained on a GaAs substrate. Because of the large miscibility gap of (GaIn)(NAs) the understanding of possible phase separation effects and of the structure formation process of the multi-quantum well

(MQWs) is of key importance to achieve controlled epitaxial growth. We have investigated the microstructure of layer systems with up to 38% In and up to 5% N using high resolution transmission electron microscopy. Applying low-temperature MOVPE growth, high quality compressively strained (GaIn)(NAs)/GaAs-MQW structures are realized. The roughness of the interfaces is in the order of some monolayers. However, increasing the N content to 4.5% results in a deterioration of the layer structures. These morphological changes are presumably caused by microscopic strains and result in the formation of trapezoidal-, dot- and cusp-like features in the wells. These observations will be correlated to microscopic and macroscopic strain states of the quaternary (GaIn)(NAs).