SYMPOSIUM I

Self-Organized Processes in Semiconductor Alloys– Spontaneous Ordering, Composition Modulation, and 3-D Islanding

November 29 – December 2, 1999

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* Invited paper

SESSION I1: QUANTUM DOTS - I
Chairs: Bruce A. Joyce and Ray D. Twesten
Monday Morning, November 29, 1999
Wellesley (M)

8:30 AM I1.1
MOLECULAR BEAM EPITAXY STUDY OF 3D ISLANDING IN THE InAs/(Al,Ga)As SYSTEM. P. Ballet, J.B. Smathers, H. Yang, C.L. Workman and G.J. Salamo. Physics Dept, University of Arkansas, Fayetteville, AR.

We present the results of an investigation of the 3D islanding in the highly mismatched InAs/(Al,Ga)As system using a combined molecular beam epitaxy - scanning tunneling microscopy facility. The results give details on the 2D-3D growth mode transition as well as the density and morphology of the free-standing 3D islands. Our discussion focuses on the effect of the Al content. We give strong evidence that the chemical nature of the starting surface greatly impacts the growth of the 3D InAs islands. In particular we show that by using a pure AlAs surface it is possible to control independently the size and density of the islands. We also demonstrate that the growth of InAs on AlAs can be describe as Stransky-Krastanov as opposed to that of InAs/GaAs for which strong material reorganization occurs. Finally we discuss the potential of these islands when used as quantum dots and we give clear evidence that the composition of the (Al,Ga)As barriers can be designed to achieve large tunability of the quantum dots emission energy.

8:45 AM I1.2
THE SHAPE OF InAs SELF-ASSEMBLED QUANTUM DOTS GROWN ON InGaAs/InP. Sukho Yoon, Youngboo Moon, Tae-Wan Lee, and Euijoon Yoon, School of Materials Science and Engineering, Seoul National University, Seoul, KOREA.

The self-assembled quantum dot (SAQD) formation has attracted a lot of attention for its potential applications to future high-performance, electronic and optical devices. Since the local potential environment of the dots largely determines the electronic and optical properties of quantum dots, the detailed information on the shape as well as the compositional profile of the SAQDs is very important. Electronic structure calculations of quantum dots are currently based on the assumed dot shape. Study on the shape of the quantum dots itself gives us many clues to the energetics and kinetic pathways for the dot formation. Moreover, the precise information on the initial shape of the uncapped SAQDs is the very starting point for the full understanding on the shape evolution towards the capped SAQDs, enabling us to engineer the physical properties of the SAQD. However, the shape of III-V SAQDs is still controversial, compared to the well-defined {105}-faceted SiGe/Si quantum dots. In this study, InAs self-assembled quantum dots were grown on InGaAs/InP by metalorganic chemical vapor deposition. The relatively large dot sizes ($\sim$100 nm wide and $\sim$10 nm high) due to the smaller misfit strain compared to InAs/GaAs dots, enabled us to identify {136} facets by atomic force microscopy. Moreover, the {136}-faceted InAs dots were elongated along either [1-30] or [-310] to form parallelogram-based dots, analogous to hut clusters observed in SiGe/Si quantum dots, however, due to their unique geometry with {136} facets they looked as if they were overall elongated along [1-10] direction. We believe that these parallelogram-based dots are kinetically favored over rhombus-based dots. Some parallelogram dots were found to have a small fraction of {110} facets, presumably under shape transition towards dots with facets of higher symmetry. Detailed information on the shape and the size distribution of the {136}-faceted dots will be presented.

9:00 AM I1.3
HIGH RESOLUTION ANALYSIS OF EMBEDDED QUANTUM DOTS. Alan Harvey, UMIST, Dept of Physics; Helen Davock and Peter J. Goodhew, Univ of Liverpool, Dept of Engineering, Liverpool, UK.

A key piece of information in the modelling of quantum dot behaviour is the composition of the dot after any capping and/or annealing processes. It is important to know the composition and uniformity of the dots after they have been embedded in a semiconducting matrix which usually contains one or more of the elements in the dot. This is a classically difficult analytical problem for any TEM technique. We have developed a model of the interaction between the electron probe and any dot/wetting-layer/matrix configuration. This model predicts the shape of an analytical line scan for any particular configuration and includes the effect of beam broadening on the analysis of dots at different depths in the thin section. The results are compared with STEM analyses of InAs dots in a GaAs matrix.

9:15 AM I1.4
Abstract Withdrawn.

9:30 AM *I1.5
GROWTH PHENOMENA OF QUANTUM DOT STRUCTURES IN THE InGaAs SYSTEM INVESTIGATED BY TEM TECHNIQUES. Peter Werner, Max-Planck-Institut für Mikrostrukturphysik, Halle/Saale, GERMANY.

Semiconductors having structures of reduced dimensions as, e.g., quantum dots (QDs) are expected to exhibit special optical and electronic properties leading to a new kind of opto-electronic devices. In the past 15 years, the generation of QDs has been attempted using different techniques. However, there was a breakthrough recently initiated by employing self-ordering mechanisms during the epitaxial growth of lattice-mismatched semiconductor alloys forming 2-dimensional and 3-dimensional arrays of coherent islands based on the "Stranski-Krastanow" growth mode. The applicability of such quantum structures can further be improved by using stacked layers instead of single layers of QDs.
The contribution is mainly focused on the formation and properties of InGaAs islands ("dots") in a GaAs matrix, viz. a system showing properties similar to those of other materials systems. Depending on the growth techniques applied (MBE or MOCVD), the islands/dots differ in size, shape, chemical composition, and lattice strain. The goal of investigating these systems, especially the QD layers, by transmission electron microscopy (TEM) is to reveal the correlation between the morphology/structure and the optical behavior of these systems (photoluminescence, cathodoluminescence). As an example, the QD shape (pyramidal or spherical islands) has a strong influence on the electronic states. A technological application of such 3D structures are QD lasers emitting light in the infrared region. While at first such lasers emitted light in the range of 1.1μm, the development is directed to structures emitting light at 1.3 μm and 1.5 μm at RT. The talk will point out some structural/growth possibilities to reach this goal.
TEM imaging techniques used for such structural analyses will be described, including conventional diffraction contrast and HREM, respective examples of which will be presented. For the chemical analysis GIF/PEELS are appropriate methods. Applications and limitations of such investigations will be discussed.

10:30 AM *I1.6
SPECTROSCOPY OF SELF-ORGANIZED QUANTUM DOTS WITH BIAS-CONTROLLED ELECTRON OCCUPATION. Lars Samuelson, Dan Hessman, Jonas Persson, Mats-Erik Pistol, Craig Pryor and Werner Seifert, Lund Univ, Solid State Physics/Nanometer Structure Consortium, Lund, SWEDEN.

Macro- as well as micro-photoluminescence studies of InP/GaInP quantum dots (QDs) fabricated via the Stranski-Krastanow growth mode always show multiple luminescence lines, with an unexpected spectral width, even for an individual QD[1]. The origin of this unusual behavior has been debated and until now no clear picture has emerged. We have recently developed a new spectroscopic tool with which we can follow the luminescence of a single QD during the application of an electric field using a transparent Schottky barrier on the surface of the GaInP barrier material. This enables us to follow the evolution of each of the peaks as a function of applied bias. With applied negative bias the Fermilevel is shifted to lower energies and individual lines in the multiplet sequentially disappear, starting from the high-energy side, as one after one of the excited states in the QD are de-populated. For negative biases such that only a few electrons are still present in the QD we observe that the originally 1-2 meV broad lines split up into several very sharp lines, with FWHM values comparable to the resolution of our spectroscopic system (50-100 eV). In the extreme limit of de-population we detect what we believe is an isolated electron-hole pair. In the other limit of flat-band conditions we estimate that 15-20 electrons occupy the QD, leading to the multiplet of lines over the spectral range of 40-45 meV. This estimation is based on electronic structure calculations for the bound states in the InP QDs, which predict that in this energy range exist approximately 8-10 doubly occupied states [2]. A self-consistent picture is finally obtained when one applies the electrostatic repulsion per added electron, which from capacitance spectroscopy has been estimated to be around 10 meV/electron [3]. In conclusion, we present an intriguing QD system which allows controlled tuning of the occupancy of a single QD in the range 0 20 electrons, in contrast to InAs/GaAs QDs for which only about two electrons can be bound. This makes us think that these QDs may not only mimic properties of atoms but may actually allow studies that go beyond the atomic picture in that we have a knob by which we may tune the occupancy of a single, artificial, atom. References: [1] Hessman et al., APL 69, 749 (1996) [2] Pryor et al., PRB56, 10404 (1997) [3] Anand et al., APL 67, 3016 (1995)

11:00 AM I1.7
THE EFFECT OF INTERMIXING ON SELF-ASSEMBLED QUANTUM DOT FORMATION. Hawoong Jeong, Albert-Laszlo Barabasi, University of Notre Dame, Department of

Physics, Notre Dame, IN.

Intermixing is known to affect both the the size and the density of the self-assembled quantum dots (SAQD). Here we develop an equilibrium theory to investigate the effect of alloying on the island characteristics. We show that when alloying is present, some phases, believed to describe the formation of SAQDs, are absent. We discuss how does the degree of alloying affect the phase diagram of SAQD formation. Finally, the results are compared with high temperature growth experiments, exhibiting intermixing and alloying during the formation of strained islands.

11:15 AM I1.8
CHARACTERIZATION OF InAs QUANTUM BOXES USING CROSS-SECTIONAL SCANNING TUNNELING MICROSCOPY. Bernard Legrand, B.Grandidier, Jean Philippe Nys, Yahn Michel Niquet, Didier Stievenard, Jean Michel Gerard and Veronique Thierry-Mieg.

Cross-sectionnal scanning tunneling microscopy images and scanning tunneling spectroscopy results on InAs quantum dots grown on GaAs are presented. The images reveal the vertical self-alignment of the dots, the roughness of the dot interfaces and the strain distribution along the growth direction. The pairing probability versus the volume of dots and the distance between two successive arrays of dots is modelised using a 2D analysis. Finally, local spectroscopy evidences the electronic confinement in the dots, and the density of electronic states associated with the fundamental and the first energy levels of a dot are also presented.

11:30 AM I1.9
InAs QUANTUM DOTS ON SILICON. L. Hansen, F. Bensing, A. Ankudinov[1], A. Waag, Experimentelle Physik III, Universitaet Wuerzburg, GERMANY; [1]on leave from Ioffe Institute, St.-Petersburg, RUSSIA.

Embedding of photoactive direct bandgap III-V materials into silicon is interesting for optoelectronic applications. Most III-V materials have a large lattice mismatch to Si, and the growth of thick layers is obstructed due to dislocation generation. Recently, thin InAs films have been grown on Si, forming an array of coherently strained QDs. Also, luminescence from the capped dots has been observed up to room temperature[1]. We present our latest results on the molecular beam epitaxy growth of InAs QDs on silicon. We observe an abrupt transition from 2D to 3D growth after the deposition of nominally 1.7 ML of InAs. The critical thickness is independent of the III/V flux ratio, wheras the density of the QDs, measured ex situ by AFM, depends strongly on the BEP(As/In) and the amount of deposited InAs. We observe a maximum of 10^{11} cm^{-2} dots of approximately 30 nm diameter and an average height of 5-6 nm. We could not prepare a 2D wetting layer. After the deposition of less than 1.7 ML of InAs, a lowering of the substrate temperature was always accompanied by a transition into a 3-dimensional phase showing QDs. In addition, by in-situ x-ray emission spectroscopy we determined the temperature stability of the capped InAs QDs. For temperatures above 350°C, a clear decomposition of InAs occurs. Further, we will report on first results of InAs QDs on Si, protected by an additional ZnTe-cap against surface oxidation, where we observe a PL peak at 1.2 -1.3 μm, a wavelength range which is very interesting for optical fibre applications.
[1]Heitz et al., Appl. Phys. Lett. **74, 1701 (1999)**

SESSION I2: SPONTANEOUS ORDERING IN SEMICONDUCTOR ALLOYS
Chairs: Satyen K. Deb and Rebecca L. Forrest
Monday Afternoon, November 29, 1999
Wellesley (M)

1:30 PM *I2.1
X-RAY AND TEM STUDIES OF ORDERING IN TERNARY SEMICONDUCTOR ALLOYS. Joseph Kulik, Univ of Houston, Texas Center for Superconductivity (TCSUH) and Dept of Physics, Houston, TX; Rebecca Forrest, Univ of Houston, Dept of Physics, Houston, TX and UCLA, Los Angeles, CA; Jianhua Li, Terry D. Golding, Simon C. Moss, Univ of Houston, Dept of Physics, Houston, TX.

Both X-ray scattering and transmission electron microscopy (TEM) may be used to study ordering (including orientational superlattice formation) and faulting - both twin and stacking disorder - in ternary semiconductor alloys of the generic form $III(1)_xIII(2)_{1-x}$-V in which [111] CuPt and 'triple period' ordering may form during epitaxial growth of thin films. We have performed studies of both GaInP and $Al_{1-x}In_xAs$ to recover the degree of order and to demonstrate the presence of both short-range order and substantial faulting. We have also initiated synchrotron X-ray studies of orientational ordering in GaInP supplied by NREL (Z. Zhang, A. Mascarenhas). In all of these studies we are concerned with the quantitative evaluation of the degree of order, and its relationship to electronic structure, and the demonstration of both faulting and effects arising from the disparity in atomic size between the group III atoms. Diffuse scattering studies form an essential component of our analysis of these materials and the X-ray and TEM techniques and interpretation will be discussed.

2:00 PM I2.2
FIRST OBSERVATION OF ATOMIC LONG RANGE ORDERING IN METAL-OXIDE BASED ZnMgO WIDE BANDGAP HETEROSTRUCTURES. R.D. Vispute, S. Choopun, D.M. Chalk, S.B. Ogale, R.P. Sharma and T. Venkatesan, CSR, Department of Physics, University of Maryland, College Park, MD; A. Iliadis, Department of Electrical Engineering, University of Maryland, College Park, MD; D.C. Look, Semiconductor Research Center, Wright State University, Dayton, OH.

Wide bandgap semiconductors have been under investigation due to their potential for short-wavelength light emitting devices. There has been a significant progress in III-nitrides that has resulted in demonstration of blue LEDs, laser diodes, and high temperature/high power electronic devices. Another material analogous to GaN is ZnO, which is a direct bandgap semiconductor with energy gap of 3.3 eV at room temperature and is being considered as a futuristic material for UV and blue light emitting devices. In this system, band gap engineering can be achieved by alloying ZnO with Mg and Cd for enlarging and narrowing the bandgap, respectively. Here, we report the first observation of atomic long range ordering in the metal-oxide based wide bandgap (3.68 eV) ZnMgO alloy semiconductor thin films grown on sapphire (0001) by pulsed laser deposition. In contrast to the cubic III-V compounds where ordering was previously observed, the ZnMgO system has the hexagonal wurtzite structure. The ordering was deduced from observations of forbidden x-ray diffraction peaks in the wurtzite structure. Under optimum growth conditions, Zn and Mg preferentially occupy hcp sublattice. The relative intensity of the superlattice peak was largest for the Mg content in the range of 10% which is about 50% of the solubility of Mg in ZnO. The ordered films also showed reduction in the bandgap of 32 meV. Influence of lattice mismatch, buffer layer, growth temperature, growth rate, oxygen pressure, and thermal annealing on the atomic long range ordering in ZnMgO and optoelectronic properties will be discussed. The observations of long range order in ZnMgO alloy semiconductor is quite important in the context of understanding issues related to the growth kinetics, surface reconstruction, phase stability of metal-oxide based heterostructures and devices. This work was supported by the NSF-UMD MRSEC (DMR 9632521) and NSF contract supervised by Dr. Khosla.

2:15 PM I2.3
EPITAXIAL GROWTH of $CuInSe_2$ IN A LAYERED-TETRAGONAL STRUCTURE. B.J. Stanbery, C.-H. Chang, S. Kincal, S. Kim, L. Li, T.J. Anderson, U. of Florida, Dept of Chemical Engineering, Gainesville, FL; G. Lippold, Institute for Surface Modification, Leipzig, GERMANY; P. Ahrenkiel and M. Al-Jassim, NREL, Golden, CO.

Migration-Enhanced Epitaxy (MEE) has been successfully employed to grow epitaxial films of $CuInSe_2$ on (001) GaAs that are ordered in a metastable layered-tetragonal structure rather than the equilibrium chalcopyrite structure. Theoretical calculations of formation energies in the Cu-In-Se material system[1] have indicated that ordering of the cation sublattice along the (001) direction in a CuAu structure is nearly isoenergetic with the chalcopyrite structure. Experimental observation of this structure over nanoscale regions in the analogous sulfide compound $CuInS_2$ has been reported in a recent TEM study[2], but never before in the $CuInSe_2$ system. Current evidence for the layered-tetragonal structure is provided by two methods. X-ray diffraction θ-2θ scans exhibit an unusually prominent series of diffraction peaks at $\theta \approx 15.45°$, 30.93°, 47.19°, 64.17° that we tentatively assign to the (002), (004), (006), and (008) reflections of the structure. Only the (008) peak is allowed for the chalcopyrite structure. Raman spectra exhibit heretofore-unreported peaks at 52, 186, and 462 cm^{-1}, in addition to the A_1 mode at 175 cm^{-1} and the B_2 (TO) mode at 232 cm^{-1}. The 52 and 186 cm^{-1} peaks are near the estimated acoustic and A_1 optical zone boundary phonon energies, respectively, of the chalcopyrite $CuInSe_2$ structure, rendered optically active by zone-folding resulting from the layered-tetragonal structure. These observations will also be supplemented with the results of ongoing TEM studies. Film growth appears to occur in a Stranski-Krastanov mode. The effects of growth conditions and overall stoichiometry on 3D island formation will be described, including the observation that their ordering into self-assembled arrays occurs only in the case of copper excess. [1]S.-H. Wei, et. al., Physical Review B 45(5), 25332536 (1992). [2]D.S. Su, et. al., 11th International Conference on Ternary and Multinary Compounds, 229-232, Salford, England, (1997).

2:30 PM *I2.4
SURFACTANT EFFECTS ON ORDERING IN GaInP GROWN BY OMVPE. G.B. Stringfellow, College of Engineering, University of Utah, Salt Lake City, UT.

CuPt ordering in semiconductor alloys is driven by the surface structure and steps are found to be important in the ordering process. Donor and acceptor impurities are well known to eliminate ordering. For many dopants, for example for Si and Zn in GaInP, the disordering is caused by an increase in the Ga/In intermixing in the bulk. However, Te is found to behave as a surfactant, with a marked effect on the step structure. The disordering due to Te occurs at much lower concentration than for Si. The increase in step velocity induced by Te is postulated to be responsible for the disordering. Perhaps the most exciting development in this area is the use of the isoelectronic group V element Sb to control the surface reconstruction and, hence, the order parameter and the GaInP bandgap energy. Modulation of the TESb flow rate during the growth cycle has been used to produce a heterostructure with a 135 meV bandgap difference between two layers having the same composition, one grown with and the other without antimony.

3:30 PM I2.5
SPATIALLY-RESOLVED PHOTOLUMINESCENCE IN SPONTANEOUSLY-ORDERED $GaInP_2$. S. Smith, H.M. Cheong, B.D. Fluegel, J.F. Geisz, J.M. Olson, L.L. Kazmerski and A. Macarenhas, NREL, Golden, CO.

The low-temperature (5K) photoluminescence (PL) of partially-ordered $GaInP_2$ is spatially resolved using high-resolution ($\sim 0.7\mu$m) scanning optical microscopy combined with high-resolution spectroscopy ($\sim 40\mu$eV), revealing the spatial variation in band gap energy and the spatial origin of the ordering-induced low-energy emission and the associated 'quantum-dot-like' narrow spikes which appear when examining areas smaller, or of comparable size, than a single ordered domain. The large number of spectra taken within a micron-sized area allow a detailed look at the statistical variation in band-gap energy and lineshape. A systematic study of a series of samples where the order parameter varies from $\eta \sim 0$ to 0.45 shows that for the mostly highly-ordered samples, the statisitical distribution of excitonic energy and linewidth show evidence of exciton localization, which is also clearly seen by examining the spatial maps of the excitonic energy and linewidth extracted from the measured spectra.

3:45 PM *I2.6
CORRELATION OF InGaP(001) SURFACE STRUCTURE DURING GROWTH AND CuPtB-TYPE BULK ORDERING. M. Zorn, J.-T. Zettler, W. Richter, Institut für Festkörperphysik, Technische Universität Berlin, Berlin, GERMANY; A.I. Shkrebtii, Department of Physics, University of Toronto, Toronto, CANADA; P. Kurpas, M. Weyers, Ferdinand-Braun-Institut für Höchstfrequenz-technik, Berlin, GERMANY; B. Junno, L. Samuelson, Department of Solid State Physics, Lund University, Lund, SWEDEN.

The mechanism causing CuPtB-type ordering of InGaP grown lattice matched to GaAs is investigated by in-situ reflectance anisotropy spectroscopy (RAS/RDS) and reflection high-energy electron diffraction (RHEED). Experiments have been performed both in metal organic vapour phase epitaxy (MOVPE) and in chemical beam epitaxy (CBE). Additionally, total energy calculations have been performed for differently ordered InGaP slabs terminated by different surface reconstructions. In the experiments, first the bulk contribution to the reflectance anisotropy, caused by the loss of symmetry due to CuPtB-type bulk ordering, was determined. Therefore, the superimposed surface contribution to the RAS spectra could be extracted, which was identified for all growth conditions (varying temperature, growth rate, doping level, and sample off-orientation) as a superposition of only two characteristic types of spectra corresponding to a (2x1) and (2x4) surface reconstruction, respectively. Bulk ordering only occurs when InGaP growth is performed under phosphorous-rich (2x1)-like surface conditions and it completely disappears when changed growth conditions cause a less-phosphorus-rich (2x4)-like surface dimer configuration no matter which specific growth parameters is changed. The P-dimers in (2x1) symmetry at the growth surface trigger the bulk ordering driven by an energy gain of 0.26 eV/ surface atom according to the TE calculations.

4:15 PM I2.7
DOMAIN SHAPE ANALYSIS OF CuPt-B ORDERED GALLIUM INDIUM PHOSPHIDE. C.D. Moore, R.R. Hess, R.L. Forrest, and M.S. Goorsky, Dept of Materials Science, University of California, Los Angeles, CA.

Reciprocal space mapping using high resolution x-ray diffraction has been used to study the size and distribution of ordered domains in CuPt-B ordered $Ga_xIn_{1-x}P$ grown by metalorganic vapor phase epitaxy. Our technique maps each ordered reciprocal space point along different crystallographic directions and this provides three dimensional information about the ordered domains and helps distinguish among mosaic spread, domain shape, and finite size peak broadening effects. These competing contributions hinder analysis using more conventional double axis diffraction measurements. The difference in beam size and beam coherence width - in comparison with transmission electron microscopy - allows more detailed crystallographic information about the structure of larger domains to be obtained. Maps of the ordered domains from ~ 1 μm GaInP grown on GaAs tilted 2 degrees toward [1 0 0], with uniform domain microstructure, show two {111} variants with order parameters of about 0.20 and 0.018. The shape of the $\frac{1}{2}$ ($\bar{1}$ 1 5) crystal truncation rod has a circular cross section; this is the same shape that is observed from transmission electron diffraction patterns taken along the same crystallographic direction. 10 μm GaInP, grown on GaAs tilted 6 degrees toward the [$\bar{1}$ 1 0], show reciprocal space maps that represent domains elongated and tilted by a few degrees from the [0 0 1] growth direction. Three-dimensional mapping indicates that the ordered domains are more extended along the [1 1 0] than the [$\bar{1}$ 1 0] direction. Domain morphology will be discussed in terms of growth kinetics and substrate miscut.

4:30 PM *I2.8
CuPt ORDERING SIGNATURES OF PHONONS IN $GaInP_2$. Francesc Alsina, Univ Autonoma de Barcelona, Dept of Physics, Bellaterra, SPAIN; Hyeonsik M. Cheong, National Renewable Energy Laboratory, Golden, CO; Narcís Mestres, ICMAB-CSIC, Bellaterra, SPAIN; Angelo Mascarenhas, National Renewable Energy Laboratory, Golden, CO; Jordi Pascual, Univ Autonoma de Barcelona, Dept of Physics, Bellaterra, SPAIN.

During the following ten years after spontaneous ordering was first observed in the $GaInP_2$ alloy most of the studies on optical properties were focused on analyzing the influence of ordering on the electronic states. The changes induced by ordering in lattice dynamics were found less sensitive and thus the studies on the optical properties of phonons were more scarce. In the last few years, the growth of strongly ordered single variant $GaInP_2$ samples has permitted us to gain a remarkable amount of experimental evidence for ordering effects on the phonon spectra.
In this communication we present a comprehensive overview of spectroscopic measurements of phonons in ordered $GaInP_2$. The major signature of CuPt ordering in the Raman spectra is the emergence of new peaks in both the acoustic and the optical regions. Concerning the measurements in the infrared spectrum, anisotropy effects in the optical region are manifest. At present, a definitive picture of the influence of ordering on the vibrational properties has not yet been achieved. From the experimental side, two main drawbacks prevent a reliable phonon modes assignment: (a) nowadays samples are only partially ordered, and (b) it is difficult to establish a complete account of the selection rules.

SESSION I3: QUANTUM DOTS - II
Chairs: Anupam Madhukar and Frances M. Ross
Tuesday Morning, November 30, 1999
Wellesley (M)

8:30 AM I3.1
SELF-ASSEMBLED InAlP/GaP QUANTUM DOTS GROWN BY MOCVD. Jae-Hyun Ryou, Uttiya Chowdhury and Russell D. Dupuis, The University of Texas at Austin, Microelectronics Research Center, Austin, TX; Chavva V. Reddy and Venkatesh Narayanamurti, Harvard University, Division of Engineering and Applied Sciences, Cambridge, MA; David T. Mathes and Robert Hull, The University of Virginia, Department of Materials Science and Engineering, Charlottesville, VA.

We have grown self-assembled $In_xAl_{1-x}P$ (x=0.6-1.0) quantum dots (QDs) embedded in GaP cladding layers using low-pressure metalorganic chemical vapor deposition (LP-MOCVD). $In_xAl_{1-x}P$ QDs are grown in the Stranski-Krastanow (S-K) mode on a GaP buffer layer and substrate with various substrate tilt-angles toward <111>B and <110>. QD formation was studied under various growth conditions, such as flow rates of III elements, V/III ratios, growth temperatures (500-700°C), and growth sequence. The QDs were grown in an EMCORE GS3200 reactor using triethylgallium, trimethylindium, and trimethylaluminum as group-III precursors and PH_3 for the group-V precursor. The flow rates for the group III precursors were reduced in order to achieve monolayer control of the growth rate for the growth of $In_xAl_{1-x}P$ QDs. Atomic force microscopy (AFM) was performed to investigate the onset of strain-induced 3-D island growth and the size, distribution, and density of bare QDs. The onset of 3-D growth depends on the

substrate tilt direction and angle. According to the AFM images, the average dot size varied from 3 nm to 20 nm in height, depending on growth conditions. Under optimized growth conditions, high-density, highly uniform arrays of QDs were formed. Scanning tunneling microscopy (STM) images confirmed the AFM data. Ballistic electron emission microscopy (BEEM) was employed to measure the band structure properties at InAlP-GaP interfaces and the QDs. Also, high-resolution transmission electron microscopy (HR-TEM) was performed to observe the cross sectional view of the InAlP QDs embedded in GaP and to study the composition and uniformity of the dot material.

8:45 AM I3.2
ENERGY ANALYSIS FOR HETEROEPITAXIAL FILM-SUBSTRATE SYSTEMS WITH AN ARRAY OF SELF-ASSEMBLED QUANTUM DOTS. Cheng-hsin Chiu, Institute of Materials Research and Engineering, SINGAPORE.

The nano-structure of self-assembled quantum dots, fabricated by the Stranski-Krastanow growth mode of heteroepitaxial film-substrate systems, has been a subject under extensive discussion in the literature recently. Remarkable progress has been made in understanding the morphological evolution of the heteroepitaxial systems from a theoretical point of view; however, the progress is still limited to some special cases. For example, the island shape is presumed, some of the important energetic forces acting on the systems are ignored, or there are only a small number of islands in a calculation cell. These constraints in analysis have impeded researchers from having a general picture about the self-assembly process. The problem motivates us to develop a perturbation method, within the framework of continuum mechanics, for investigating the free energy of a heteroepitaxial system with an array of dots on the surface. The method provides an efficient way for determining how the free energy varies with the structure of the quantum dot arrays, such as the island morphology, the island density, the island size, and the wetting layer thickness. And the method can take into account all the important energetic forces acing on the heteroepitaxial system. The forces include the mismatch strains between the film and the substrate, the surface energy anisotropy, the surface stress, and the film-substrate interaction. The method makes it possible to develop a clear picture about the whole self-assembly process, ranging from the nucleation of the quantum dots to the morphological evolution of the dot array. The picture explains well the important experimental findings such as the Stranski-Krastanow transition, the surface roughening process, the formation of facet islands, the hut-dome transition, and the bimodal distribution of the island sizes. The picture also sheds some light on the effects of material properties on the stability of the island array against coarsening.

9:00 AM I3.3
INTERDIFFUSION AND SEGREGATION IN STACKED InAs/GaAS QUANTUM DOTS. B. Lita, R.S. Goldman, Dept of Materials Science and Engineering, University of Michigan, Ann Arbor, MI; J.D. Phillips, P.K. Bhattacharya, Dept 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 (3D) dot lattices, which have novel electronic and optical properties. Although highly ordered arrays have been achieved in a number of materials systems, the atomic-level limitations to the perfection of the dot lattices are not fully understood. Therefore, we have investigated the atomic scale details of interdiffusion and segregation in stacked self-assembled InAs/GaAs quantum dots. Using ultra high vacuum (UHV) cross-sectional scanning tunneling microscopy (XSTM), we have observed lateral variations in the vertical positions of In atoms in both the stacked dots and wetting layers. By counting In and Ga atoms, we have determined the In profile along the growth direction, and obtained vertical In-Ga interdiffusion and 1/e surface segregation lengths of 1.25 and 2.8 nm, respectively. We also observe significant vertical intermixing in dot stacks. Since In atoms are often observed on top of the last dot in a stack, but none are observed below the first dot, In surface segregation is the dominant mechanism of vertical coupling between the stacked quantum dots. Occasional interruptions of the wetting layer due to post-growth diffusion and/or segregation processes are apparent. Such lateral diffusion and/or segregation processes in the wetting layer may also affect the lateral spacing between columns of dot stacks, thereby providing a means of producing ideal 3D arrays of stacked quantum dots.

9:15 AM I3.4
THE STRUCTURE OF CAPPED AND UNCAPPED InAs/GaAs QUANTUM DOTS. Dan Zhi, D.W. Pashley*, Centre for Electronic Materials and Devices, The Blackett Laboratory, Imperial College, London, UNITED KINGDOM, *Department of Materials, Imperial College, London, UNITED KINGDOM.

The optoelectronic properties of quantum dot (QD) devices are influenced essentially by the size, shape, arrangement, crystal morphology, and chemical composition of QDs. During the capping process the difference of the atomic size between the QD and the capping layer produces, by necessity, strain. Thus the electronic structure of these dots is controlled not only by the size effect but also by strain. The capping process also change the QD shape and the composition. In the present study, single layer InAs/GaAs (001) QD structures with different thickness capping layers were fabricated by MBE growth. The different techniques of transmission electron microscopy (TEM), including diffraction-contrast and high-resolution lattice images as well as analytical electron microscopy (AEM), were used to characterize both the microstructure and microchemistry down to the atomic scale. The multifacet nature of uncapped QDs was revealed by HRTEM images. The {113} facets which were observed along the [1-10] zone axis were shown to contain {111} growth steps. The lattice spacing changes and tetragonality within the QD, which are due to the misfit with the GaAs substrate, were used to measure the local composition/lattice strains. Coalescence of some adjacent QDs was found by HRTEM, following the lateral spreading of the QDs during the initial stages of capping. The atomic scale details obtained by HRTEM are combined with the results of reflection high energy electron diffraction (RHEED), field-emission gun scanning transmission electron microscopy (FEG-STEM), and high resolution X-ray diffraction (HRXRD) to provide information on the structure of the QDs and the capping process.

9:30 AM *I3.5
STRESS, SURFACE KINETIC PROCESSES, METASTABILITY, AND SELF-ORDERING IN SEMICONDUCTOR EPITAXY. Anupam Madhukar, University of Southern California, Departments of Materials Science and Physics, Los Angeles, CA.

A variety of phenomena in semiconductor epitaxy uncovered and examined in the past two decades or so have firmly established the ubiquitous nature of stress dependent surface kinetic processes and their synergistic role in controlling the formation of metastable structures with unique physical properties. This talk will utilize illustrative experimental findings from growth profile evolution, strain relaxation, and alloy segregation in growth on planar and patterned substrates with a view to evolving an atomistic kinetic framework that provides a deeper understanding of the phenomena and helps guide the development of new approaches to creation of semiconductor nanostructures.

10:30 AM I3.6
CROSS-SECTIONAL SCANNING TUNNELING MICROSCOPY STUDIES OF SIZE, SHAPE, STRAIN, AND COMPOSITION PROFILE OF SELF-ASSEMBLED InGaAs QUANTUM DOTS. Ning Liu, Chih-Kang Shih, The Univ of Texas at Austin, Dept of Physics, Austin, TX; Oleg Baklenov, Archie L. Holmes Jr., The Univ of Texas at Austin, Dept of Electrical and Computer Engineering, Austin, TX.

We report cross-sectional scanning tunneling microscopy (XSTM) studies of InGaAs self-assembled quantum dots (QDs) grown using migration enhanced epitaxy (MEE). Samples were cleaved in-situ to reveal either (110) or $(1\bar{1}0)$ cross-sectional surfaces. For the 10 ML QDs, they exhibit truncated-pyramid shapes with well-defined facets on both (110) and $(1\bar{1}0)$ projections. On the (110) surface, the orientation of the facets is about 35 degrees with respect to the base of the QDs, and on the $(1\bar{1}0)$ surfaces it is about 25 degrees with respect to the base. The average height of the 10 ML QDs is about 10 nm, while the average base length is about 45 nm along the (110) projection and about 61 nm along the $(1\bar{1}0)$ projection. Most importantly, the composition appears highly non-uniform, with an In-rich core having an inverted-triangle shape. Similarly, the distribution of the lattice parameters (as determined from the STM) within and around the QD is also inhomogeneous consistent with an inverted-triangle shape of In-rich core in the QD.

10:45 AM I3.7
NON-UNIFORM ALLOY COMPOSITION WITHIN QUANTUM DOTS. J. Tersoff, IBM Watson Center, Yorktown Heights, NY.

In heteroepitaxy, misfit strain leads to formation of islands. When capped, these may serve as self-assembled quantum dots. However, recent experiments by Ning Liu et al. show clearly that the composition within the quantum dot is highly non-uniform. As a result, the effective shape of the quantum dot (i.e. of the confining potential for electrons and holes) is radically different than the nominal shape of the island. This talk will present theoretical results explaining the observed composition profile in terms of 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 the experiment. The effect of capping on the composition and shape of the dot will also be discussed.

11:00 AM I3.8
VERTICAL AND LATERAL CORRELATIONS IN SELF-ORGANISED QUANTUM DOT SUPERLATTICES.
G. Springholz, M. Pinczolits, V. Holy, G. Bauer, Institut fuer Halbleiterphysik, University of Linz, AUSTRIA.

The formation of vertical and lateral correlations in quantum dot superlattices has proven as a means for improving the size homogeneity of the self-assembled quantum dots. These correlations are formed due to the elastic interactions between the dots on the growing surface and the already burried dots in the previous superlattice layers. Here it is shown that the elastic anisotropy play a crucial role for the formation of these correlations. In particular it is shown that correlations inclined to the growth directions may be formed if the surface normal orientation is parallel or near an elastically soft direction, and that also a most efficient lateral ordering occurs in this case (1). This is illustrated by the experimental observation of a fcc-like ABCABC vertical dot stacking sequence and nearly perfect hexagonal lateral ordering (2) in the PbSe/PbEuTe (111) superlattice system.
1. V. Holy, G. Springholz, M. Pinczolits and G. Bauer, Phys. Rev. Lett., in print.
2. G. Springholz, V. Holy, M. Pinczolits and G. Bauer, Science 282, 734 (1998).

11:15 AM I3.9
InAs QUANTUM DOTS IN A Si MATRIX: GROWTH AND PROPERTIES.
George E. Cirlin, Nikolai K. Polyakov, Vasilii N. Petrov, Institute for Analytical Instrumentation, St. Petersburg, RUSSIA; Dmitrii V. Denisov, Boris V. Volovik, Victor M. Ustinov, Zhores I. Alferov, A.F. Ioffe Physico-Technical Institute, St. Petersburg, RUSSIA; Nikolai N. Ledentsov, Robert Heitz, Dieter Bimberg, Technical University, Berlin, GERMANY; Nikolai D. Zakharov, Peter Werner, Max-Plank-Institute for Microstructure Physics, Halle, GERMANY.

Self-organisation effects at semiconductor surfaces during MBE attract strong interest during the last decade. In this research the most attention was paid to quantum dots (QDs) in III-V - III-V (e.g. InAs-GaAs), II-VI - II-VI (e.g. CdSe in ZnSe) or IV-IV (Si-Ge) materials systems. The last system attracted much attention because silicon remains a key material in modern semiconductor industry. For optoelectronic applications silicon is not suitable because of its indirect band gap nature. Attempts to improve the situation using SiGe-Si QDs did not led to significant progress as these nanostructures provide indirect band alignment both in k- and in real space. In order to increase luminescence efficiency of silicon-based structures we propose to insert direct bandgap InAs QDs in a Si matrix using MBe growth. Small coherent InAs islands additionally offers a possibility to overcome the problems of strong lattice mismatch and formation of antiphase domains inherent for the growth of thick III-V epilayers on Si. We have found that under certain growth conditions InAs/Si heteroepitaxial growth proceeds via Stranski-Krastanow or Volmer-Weber growth modes depending on the growth parameters. The critical thickness at which three dimensional InAs islands start to appear on the Si(100) surface is within the range of 0.7 - 5.5 monolayers. Their size depends critically on the growth conditions and is between 2 nm and 80 nm (uncapped islands). We have found that the critical lateral size of the coherent dislocation-free island is equal to 2 - 8 nm depending on the island height. Islands having larger size are dislocated. Annealing of the samples with InAs QDs capped with a several-nm-thick Si layer leads to the complete evaporation of the dislocated islands with the formation of pits, while coherent islands partially remain. For optimized growth conditions InAs QDs can be stacked in a Si matrix currently up to 6 periods. Optical properties of InAs QDs capped with Si reveal a luminescence band in the 1.3 mkm region. A pronounced excitation density dependence of the PL peak position and a decay time of order of 200-400 ns were observed. The electronic structure of InAs/Si QDs is discussed in view of available band offset information.

11:30 AM I3.10
MBE GROWTH, STRUCTURAL AND OPTICAL CHARACTERIZATION OF InAs/InGaAlAs SELF-ORGANIZED QUANTUM DOTS.
Victor M. Ustinov, Alexey E. Zhukov, Alexey R. Kovsh, Nikolai A. Maleev, Sergei S. Mikhrin, Yurii G. Musikhin, Andrey F. Tsatsul'nikov, Boris V. Volovik, Denis A. Bedarev, Mikhail V. Maximov, Nikolai A. Bert, Peter S. Kop'ev, Zhores I. Alferov, Ioffe Physico-Technical Institute, St. Petersburg, RUSSIA; Nikolai N. Ledentsov, Dieter Bimberg, Technical University of Berlin, Berlin, GERMANY.

InAs quantum dots (QD) have been shown to extend the optical emission range for III-V heterostructures pseudomorphically grown on GaAs substrates. One of the ways to achieve 1.3 micron emission from InAs QDs is to overgrow them with an In-containing alloy layer. In the present work we study structural and optical properties of InAs/In(Ga,Al)As QD structures grown by MBE on GaAs substrates using transmission electron microscopy (TEM), photoluminescence (PL), and electroluminescence (EL). We show that the main reason for the increase in the PL wavelength is the phase separation of the In(Ga,Al)As alloy stimulated by the InAs islands and the effective matrix bandgap plays a minor role. As the result of the local composition modulation, the effective volume of a QD is increased due to the enhancement of In concentration in the vicinity of the InAs island. We study how the effective thickness of InAs and InGaAs affect the crystal perfection and PL peak energy. Using the AlGaAs as a matrix also led to noticeable red shift of the quantum dot PL line as compared to the GaAs matrix. Possible reasons for this unexpected phenomenon are discussed. Characteristics of the GaAs-based vertical cavity surface emitting structures and high power CW RT edge-emitting lasers for the 1.3 micron range using these QDs will be presented.

SESSION I4: COMPOSITION MODULATION IN SEMICONDUCTOR ALLOYS

Chairs: Simon C. Moss and Gerald B. Stringfellow
Tuesday Afternoon, November 30, 1999
Wellesley (M)

1:30 PM *I4.1
KINETIC INSTABILITY OF SEMICONDUCTOR ALLOY GROWTH.
Iya P. Ipatova, Vladislav G. Malyshkin, Vitali A. Shchukin, Ioffe Institute, St. Petersburg, RUSSIA; Alexei A. Maradudin, Richard F. Wallis, University of California, Department of Physics and Astronomy, Irvine, CA.

Semiconductor alloy epitaxial films demonstrate at some temperatures the tendency to decompose into the periodic composition modulated structures. Quasiequilibrium spinodal decomposition is known in metallic alloys. Semiconductors are different, since modulated structures appear in epitaxial films in an open system in the process of growth. We suggest a concept of semiconductor alloy decomposition due to the kinetic phase transition from the growth regime of the homogeneous alloy to the growth of composition modulated structure. The kinetic instability is promoted by the drift of adatoms in the field of elastic driving forces created according to Vegard's law by frozen fluctuations of composition in already completed thickness of the film. For particular growth mechanism, we focus on step-flow growth from vapor on the vicinal to [001] surface of cubic substrate. Temperature of decomposition is shown to increase with the increase of elastic effects. The anisotropy of elastic forces is taken into account. We get the in-plain wave vectors of the most unstable mode of composition fluctuations which differ from elastically soft directions [I00] and [0I0]. It opens a possibility for formation of self organized superlattices oriented in different directions.

2:00 PM *I4.2
THE NATURE AND ORIGIN OF LATERAL COMPOSITION MODULATIONS IN SHORT-PERIOD STRAINED-LAYER SUPERLATTICES.
Andrew G. Norman, Scott P. Ahrenkiel, Helio R. Moutinho, Mowafak M. Al Jassim and Angelo Mascarenhas, National Renewable Energy Laboratory, Golden, CO; David M. Follstaedt, Stephen R. Lee, John L. Reno and Eric D. Jones, Sandia National Laboratories, Albuquerque, NM; K.Y. Cheng, Univ of Illinois, Dept of Electrical and Computer Engineering, Urbana, IL; Joanna Mirecki Millunchick, Univ of Michigan, Dept of Materials Science and Engineering, Ann Arbor, MI; Ray D. Twesten, Univ of Illinois, Center for Microanalysis of Materials, Urbana, IL.

Self-organized lateral composition modulations, which spontaneously form during the epitaxial growth of short-period strained-layer superlattices (SPS), are a promising route for the formation of quantum wire arrays and vertical superlattices, which are expected to lead to improved devices. Furthermore the significant band gap reduction associated with these lateral composition modulations opens up a new way of engineering the band gap of semiconductors whilst maintaining lattice-match to widely available substrates. We have made a detailed study of the nature and origin of these modulations in AlAs/InAs SPS grown by molecular beam epitaxy on InP substrates. The results have indicated that changing the sign of the global strain between the SPS and substrate changes the character of the modulations. SPS grown under moderate global tension exhibit modulations simultaneously along two directions close to $< 310 >$,

inclined ~27° either side of [110]. SPS grown under moderate compression exhibit modulations simultaneously along directions close to both the orthogonal < 100 > elastically soft directions. The lateral modulations in both the above cases are coupled to surface morphological instabilities that occur during growth of the SPS to relieve strain energy. Our recent work on MBE GaP/InP and GaAs/InAs SPS indicates they show similar behavior with modulations simultaneously present along two directions and a change in the orientation of the modulations with a change in the sign of the global strain. A strong temperature dependence of the occurrence of the modulations suggests that vertical In surface segregation during growth may play an important role in the formation of modulations. The lateral alloy segregation occurs by surface diffusion. Our recent work has demonstrated that by growth on suitable offcut substrates a single modulation direction can be selected, enabling greater control of the modulation process for the formation of quantum wire arrays.

2:30 PM I4.3
DYNAMICALLY STABLE GROWTH OF STRAINED-LAYER SEMICONDUCTOR SUPERLATTICES. L.E. Shilkrot, Dept. of Materials Science & Engineering, University of Michigan, Ann Arbor, MI; D.J. Srolovitz, Princeton Materials Institute, Princeton University, Princeton, NJ; J. Tersoff, IBM T.J. Watson Research Center, Yorktown Heights, NY.

Lateral composition and morphological modulations can form during the heteroepitaxial growth of misfitting multilayer films, as recently observed in InAs/AlAs, InGaP/InGaAsP, InAs/GaAs, InGaP/GaAs, and SiGe multilayers. We examine the growth of stress-driven morphological instabilities during the deposition of multilayer films. The instabilities are analyzed using continuum elasticity and first order perturbation theory. Each layer grows on the non-flat surface of the layer below it. All modulated interfaces below the growing surface contribute to the elastic part of the surface chemical potential and to the evolution of the morphology of the growing surface. Each layer has a different misfit, surface energy, surface diffusivity, growth rate and thickness and all morphological evolution occurs via surface diffusion. Morphological instabilities on adjacent layers can be simply classified as in-phase or out-of-phase. The out-of-phase perturbations result in the formation of compositionally modulated structures and may lead to the formation of regularly spaced islands. We predict the materials and growth conditions under which the propagation of the perturbation through the growing stack of multilayers can be entirely suppressed and the resulting superlattice possesses a structure of flat parallel layers with sharp distinctive interfaces.

2:45 PM I4.4
STABILITY OF PERTURBED GROWTH FRONTS TO STRESS-INDUCED MOBILITY VARIATIONS. Jennifer F. Sage, Harvard University, Department of Physics, Cambridge, MA; William Barvosa-Carter, HRL Laboratories, Malibu, CA; Michael J. Aziz, Harvard University, Division of Engineering and Applied Science, Cambridge, MA.

The effect of stress on atomic or interfacial mobilities (rather than on driving forces) has been shown to result in a kinetically-driven growth instability [W. Barvosa-Carter et al., Phys. Rev. Lett. 81, 1445 (1998).] for solid phase epitaxy of Si(001) under uniaxial compression. Here we report results of an experiment to test models for this new mechanism quantitatively by studying the instability in samples subjected to externally-imposed in-plane tensile stress. Because the predicted instability is first order in stress (instead of second order as in the energetically-driven instability), the amplitude of an interface perturbation is predicted to decay under tension and grow under compression. The evolution of rippled interfaces created artifically by lithographic techniques is being studied by optical interferometry and cross-section TEM. The results are compared to theoretical predictions and to previous experiments. Implications are discussed for the kinetics of islanding during growth from the vapor.

3:30 PM *I4.5
MORPHOLOGICAL AND COMPOSITIONAL INSTABILITIES OF STRAINED AND UNSTRAINED ALLOY LAYERS - THEORY AND EXPERIMENTS. Frank Glas, France Telecom, CNET, Laboratoire CDP, Bagneux, FRANCE.

We shall first consider the joint instability of a semiconductor alloy epitaxial layer with respect to a composition modulation coupled to a surface undulation. Two cases must be distinguished. For a lattice-mismatched layer, the elastic strain fields associated with the modulation and the undulation interact. This deeply modifies the critical parameters (temperature and wavenumber) associated respectively with each instability. In the case of lattice-matched alloy layers, the proper morphological instability disappears. However, Transmission Electron Microscopy (TEM) and X-ray microanalysis show that a modulation coupled to an undulation may also appear in this case. We shall demonstrate that some elastic coupling still exists in these layers, give a detailed calculation of their energy and discuss their stability. We shall then discuss TEM experiments where the morphological instability of strained layer superlattices was systematically studied. Growth of both tensile and compressive layers on surfaces variously disoriented with respect to (001) allowed us to investigate two debated questions: Does the morphological instability develop by bunching of steps already present on the substrate, or is there nucleation of new steps? What is the nature of the asymmetry between tensile and compressive layers? The main result is that, in these specimens at least, for layers under compression, the surface non-planarity develops by bunching of a large fraction of the original substrate steps, whereas for layers under tension facets or new steps appear.

4:00 PM I4.6
STEADY-STATE STRUCTURES IN COMPOSITION-MODULATED ALLOYS: KINETIC PHASE TRANSITION BETWEEN 1D AND 2D PATTERNS. Vitaliy Shchukin, Artem Starodubtsev, Ioffe Physical Technical Institute, St. Petersburg, RUSSIA.

We present a new non-linear continuum model for the epitaxial growth of an alloy which is lattice-matched on average to the substrate. The model describes how the surface evolves by deposition and by surface migration due to the gradient of a stress- and composition-dependent chemical potential. Contrary to linear kinetic models [1-3], where, in a growth of a lattice-matched alloy, composition instability does not lead to a morphological one, we show that the both are inevitably coupled in a non-linear regime. Composition instability creates elastic stress at the surface, and, if a modulation wavelength exceeds a critical value, the growing surface becomes unstable against undulations. Surface undulations enhance the driving force to phase separation and provide a kinetic phase transition from a 1D steady-state pattern to a 2D one. We obtain a steady-state structure of a growing alloy and construct a steady-state phase diagram in variables growth temperature - growth velocity. The phase diagram contains regions of homogeneous alloy growth, 1D steady-state pattern, and 2D steady-state pattern. We focus, particularly, on alloys of zink-blend semiconductors and show that the steady-state structure is goverened by both the cubic elastic anisotropy and the anisotropy of surface diffusion on (001) surface. Due to elastic anisotropy alone, a 1D pattern is a structure of stripes oriented in a < 100 > direction, and a 2D pattern is a square one. In the latter, alloy composition is modulated in [100] and [010] directions, whereas surface undulations occur in [1-10] and [110] directions. Surface diffusion anisotropy favors a rhombic rather than the square pattern. We discuss experimental data that reveal i) kinetic phase transitions between 1D and 2D patterns in InAlAs/InP growth and ii) a nonplanar surface modulated in [1-10] and [110] directions in GaInAs/InP growth. [1] J.E. Guyer and P.W. Voorhees. Phys. Rev. B 54, 11710 (1996). [2] F. Leonard and R.C. Desai. Phys. Rev. B 57, 4805 (1998). [3] I.P. Ipatova, V.G. Malyshkin, A.A. Maradudin, V.A. Shchukin, and R.F. Wallis. Phys. Rev. B. 57, 12968 (1998).

4:15 PM *I4.7
RECIPROCAL-SPACE ANALYSIS OF COMPOSITIONAL MODULATION IN InAs-AlAs SHORT-PERIOD SUPERLATTICES. S.R. Lee, J.L. Reno, D.M. Follstaedt, Sandia National Laboratories, Albuquerque, NM; J. Mirecki Millunchick, University of Michigan, Ann Arbor, MI; R.D. Twesten, University of Illinois, Urbana, IL; S.P. Ahrenkiel, A G. Norman, National Renewable Energy Laboratory, Golden, CO.

Quasi-periodic lateral superlattices are formed by spontaneous compositional modulation along the growth front during molecular-beam epitaxy of AlAs-InAs short-period superlattices (SPSs) on (001) InP substrates. The in-plane superlattice formed by the compositional modulation gives rise to corresponding transverse satellites about each reciprocal lattice point. We demonstrate that x-ray diffraction can be routinely used to map the local reciprocal-space structure of these lateral-superlattice satellites. The integrated intensity, spacing, orientation, and shape of the lateral satellites provide a reliable means for nondestructively detecting and characterizing the quasi-periodic lateral superlattice. Reciprocal-space mapping is applied in a parametric study of the conditions required to produce spontaneous compositional modulation during short-period superlattice growth. Variations in the degree of compositional modulation, its periodicity, and its vertical self-alignment as a function of the average composition, period, growth temperature, and growth rate of AlAs-InAs short-period superlattices are determined using reciprocal-space mapping techniques. The observed dependence of the lateral modulation on the average composition and period of the SPS are compared with some existing thermodynamic models of semiconductor alloys. Growth-temperature and growth-rate data are compared with an existing two-state surface-subsurface exchange model. The Division of Materials Sciences, Office of Basic Energy Sciences in the Office of Science of the United States Department of Energy (DOE) supported this work under contract

DE-AC04-94A185000. Lockheed Martin operates Sandia National Laboratories for the DOE. Midwest Research Institute operates The National Renewable Energy Laboratory for the DOE.

4:45 PM I4.8
THE ONSET AND CONTROL OF SPONTANEOUS LATERAL COMPOSITION VARIATIONS DURING THE GROWTH OF STRAINED ALLOY FILMS. Brian J. Spencer, University at Buffalo, Dept of Mathematics, Buffalo, NY; Peter W. Voorhees, Northwestern University, Dept of Materials Science and Engineering, Evanston, IL.

We present a theoretical description of lateral composition modulations as a steady-state growth mode for a strained A-B alloy film. The composition variations develop as a result of a coupling between the stress-driven morphological instability and a difference in the lattice parameters for components A and B. We show that if the surface mobilities of A and B are different then there is a critical deposition rate at which the instability is completely supressed. By analyzing the behavior of the system near this critical growth rate, we describe the wavelength and three-dimensional spatial pattern of lateral composition modulations. The predictions of our theory are compared with compositional modulations observed in experiments, and are discussed as a possible means for growing specific patterns of lateral composition modulations.

SESSION I5: QUANTUM DOTS - III / 3-D ISLANDING
Chairs: Robert M. Biefeld and Max G. Lagally
Wednesday Morning, December 1, 1999
Wellesley (M)

8:30 AM I5.1
MODIFIED STRANSKI-KRASTANOW MODE FOR Ge/Si (001) ISLAND GROWTH AT HIGH TEMPERATURES. Xiaozhou Liao, Jin Zou, David J.H. Cockayne, The University of Sidney, Australian Key Centre for Microscopy and Microanalysis, NSW, AUSTRALIA; Jie Qin, Zuimin Jiang, Xun Wang, Fudan University, Surface Physics Laboratory, Shanghai, CHINA; Rosa Leon, California Institute of Technology, Jet Propulsion Laboratory, Pasadena, CA.

Ge islands grown at 700°C on (001) Si by molecular beam epitaxy were investigated using cross-section transmission electron microscopy. An alloying process, involving mass transport from the substrate to the islands during the island growth, was identified. It was found that, as a result of Si mass transport to the Ge islands, the island/substrate interface moves towards the substrate, and trenches form on the substrate surface around the islands. Based on the above experimental observation, a modified Stranski-Krastanow (S-K) mode is proposed: In classical S-K growth, layer by layer growth takes place at the initial stage of Ge deposition, followed by island growth. The formation of small coherent islands only partially releases the misfit strain. With the growth of the island, misfit strain builds up. The strain energy is then further reduced by lowering the lattice misfit between the island and the substrate which results from the alloying of Si into the Ge island; Si is transported by surface migration because of a smaller activation energy than for bulk migration. As a result, a trench forms around the island. The subsequent island expansion necessarily starts from the bottom of the trenches and the lateral Si migration process continues as the island grows. Besides three dimensional island growth and the formation of misfit dislocations at the interface, alloying is another way to release the misfit strain. However, since the mass transport is kinetically limited by the surface migration coefficient, alloying can only be observed at sufficiently high growth temperatures.

8:45 AM I5.2
FROM KINETICS TO THERMODYNAMICS: GROWTH TEMPERATURE DEPENDENCE OF SELF-ASSEMBLED InAs QUANTUM DOT FORMATION ON GaAs(001). J. Yuan, G.D. Lian, G.H. Kim, D.A. Ritchie, Z.Y. Li, L. M. Brown, Cavendish Laboratory, Cambridge, UNITED KINGDOM.

The growth mechanism of self-assembled quantum dots on lattice mismatched semiconductor substrate is still a matter of debate. Energetic models, assuming thermal equilibrium, are successful in describing why the three-dimensional growth is favourable over two-dimensional layer-by-layer growth in films thick than one monolayer and in providing a mechanism for observed narrow size distribution of the resulting quantum dots. However, recent experiments have shown that the dot property can be remarkably insensitive to the conditions of strain in the system. Evidences are mounting that kinetic factors can also account for many observations. Since kinetic factors can be tuned, we have investigated the molecular beam epitaxy (MBE) growth of the InAs quantum dots on GaAs(001) surface as a function of deposition temperature by transmission electron microscopy. We found that, as the temperature increases, the dot size increases and dot nucleation density decreases. This is typical of growth by diffusion-limited aggregation. At the highest temperature studied (540°C), the dot size distribution narrows as predicted by the thermodynamic argument. Together with the appearance of incoherent particles, it is a sign that the growth is transformed from kinetically to thermodynamically driven. Our result indicates that many published results can be reconciled by the scale of growth temperature. We will discuss our results in terms of current models for coherent quantum dot growth. We show that the monoatomic surface steps can be used to partition the catchment area for InAs dot growth in the diffusion-limited growth. With proper preparation, regular spaced terraces on GaAs(001) surface can be used to promote linear alignment of quantum dots. When such a regular array of quantum dots are embedded in the middle of modulation doped GaAs quantum dots, the transport properties of the two-dimensional electron gases show strong anisotropy caused by dot alignment.

9:00 AM I5.3
NOVEL STM PROBE ASSISTED SITE-CONTROL OF QUANTUM DOTS WITH NANOMETER PRECISION. Hitoshi Nakamura, Shigeru Kohmoto, Tomonori Ishikawa* and Kiyoshi Asakawa ,The Femtosecond Technology Research Association (FESTA), Tsukuba, Ibaraki, JAPAN; * NEDO Industrial Technology Fellowship Researcher.

Nanometer-scale site-control of III-V semiconductor quantum dots (QDs) enables us to create new electronic and optoelectronic devices as well as new physical phenomena. Although several approaches have been performed to control site of the QDs, they could not realize the nano-scale control so far. In this paper, we propose a novel site-control technique of strained QDs formation, which can locate a QD at any required position with nm-level precision, thus providing us the artificial nano-scale arrangement of each QD. For this purpose we have developed nano-lithography and nano-site fabrication techniques for a strained QD by use of a UHV STM/MBE multi-chamber system. A nano-scale deposit was formed on a GaAs surface when relatively high voltage and current pulses are applied between the surface and a tungsten tip of the STM. Because the deposit could act as a nano-mask, the following GaAs growth formed a nano-hole just above the deposit. Then, 1.1 monolayer InAs supply produced a QD on the hole site which could act as the favorite site for the strained QD. Undesirable Stranski-Krastanov QDs were not observed at an off-site region. Using this technique, we successfully demonstrated a 100 nm-pitch array of paired 30 nm-diameter-QDs with 15 nm separation. The demonstration showed the smallest spacing between QDs reported so far in intentionally site- controlled QDs and the realization of arbitrary configuration of QDs. Therefore, the site-control technique described here will provide us a large possibility to realize new optoelectronic devices. This work was supported by NEDO within the framework of the Femtsecond Technology Project.

9:15 AM *I5.4
STRAIN ENGINEERING OF NANOSCALE STRUCTURES IN THE Ge/Si SYSTEM. Max G. Lagally, University of Wisconsin-Madison, Madison, WI.

Many current electronic devices involve the use of strained semiconductor thin films. Strain engineering can also be used for fabricating three-dimensional nanostructures by strain-induced self-assembly and self-organization. We discuss recent studies of the influence of strain on growth and ordering processes in Si and SiGe thin films, grown by CVD and MBE on macroscopic as well as patterned Si(001) and SOI (001). Using force and tunneling microscopies and low-energy electron microscopy, we characterize surface strain fields and surface/interface structures and morphologies, as well as the effect of strain on nucleation and growth. The lattice strain induces formation of ordered arrays of three dimensional islands with remarkable spatial and size uniformity, providing a potentially attractive route to fabricating novel devices involving arrays of quantum dots. We also discuss theoretical analyses and simulations based on elastic models to elucidate formation and self-organization processes driven by strain relaxation.

10:15 AM *I5.5
STRUCTURAL AND MORPHOLOGICAL SURFACE EVOLUTION OF LAYERS GROWING UNDER STRAIN. I. Goldfarb and G.A.D. Briggs, Univ of Oxford, Dept of Materials, Oxford, UK.

Understanding the factors affecting surface roughening in heteroepitaxy is equally crucial for obtaining flat high quality epilayers in planar device technology, and for controlled self-assembly of low-dimensional nanostructures. We have investigated the effects of the magnitude and sign of mismatch strain on the evolution of surfaces during heteroepitaxial growth by growing Si-Ge alloys with varying Ge content, and metal-semiconductor compounds with a purpose-selected lattice constant. With the former we varied the amount of compressive strain in the Stranski-Krastanow epilayer, while the latter, e.g. cobalt disilicide, represented the case of a

Volmer-Weber growth under tension. We have also experimented with various degrees of the substrate perfection. In-situ analysis was carried out mainly by scanning tunneling microscopy (STM), mostly in real-time, and reflection high energy electron diffraction (RHEED). Growth on the nominally flat Si(001) substrate has resulted in the formation of nanocrystals in all of the above cases, with different shapes, size-distributions, and degrees of thermodynamic stability. The similarities emphasize the importance of surface and interface energy contribution to the overall energetic balance, while some of the differences, e.g. in size-distributions, are driven by kinetics. Reactive epitaxy of cobalt silicide onto a vicinal Si(001) surface has lead to a more two-dimensional growth. This work demonstrates the ability to intentionally modify the growing surface morphology by careful selection of the deposition

10:45 AM I5.6
EVALUATION OF THE STRAIN FIELD INSIDE AND AROUND GROWTH ISLANDS BY MEANS OF X-RAY DIFFUSE SCATTERING. Thomas Wiebach, Martin Schmidbauer, Helmut Raidt, Peter Schaefer, Rolf Koehler, Wolfgang Neumann, Holm Kirmse, Michael Rabe, Fritz Henneberger, Institut fuer Physik, Humboldt-Universitaet zu Berlin, Berlin, GERMANY; Herbert Wawra, Institut fúr Kristallzuechtung, Rudower Chaussee, Berlin, GERMANY.

One of the key parameters of nanoscale islands is the strain distribution inside islands and in their vicinity. As we could already demonstrate x-ray diffuse scattering gives valuable information on the mean strain and, especially, on the strain distribution in SiGe-islands exhibiting base widths of about 100 nm. We were also able to detect a spatial distribution of the Ge-content in these islands. Additionally the strain distribution around such islands is detected by means of the diffuse x-ray scattering in the vicinity of the reflection of the host lattice. The strain distribution inside and around the islands is evaluated by comparison of experimental and simulated maps of diffuse scattering. One of the problems of this technique is that diffuse scattering contains information on shape and strain. Because the extension in reciprocal space of the shape related part of diffuse intensity inversely scales with the size of the islands, the evaluation of strain becomes the more difficult the smaller the islands are. This can be roughly characterized by the product of misfit (island-host) and size (say base width). E.g. for a Ge-island on Si (misfit 4%, base width about 30 nm) strain still significantly influences diffuse scattering and can be thus evaluated. For very small islands the strain state can be derived from the strain field surrounding the island. This will be discussed on the basis of selected examples ranging from comparatively large SiGe/Si islands (base width: about 100 nm) to small CdSe quantum dots in ZnSe/GaAs (base width: about 15 nm). In the latter case the results are compared with transmission electron microscopy data.

11:00 AM I5.7
NOVEL STRAIN-RELIEF MECHANISMS FOR Ge/Si(100) COHERENT ISLANDS. Jeff Drucker, Sergio Chaparro, Y. Zhang, Physics Department, The University of Texas at El Paso, TX; D. Chandrasekhar, M.R. McCartney and David J. Smith, Center for Solid State Science, Arizona State University, AZ.

We identify novel strain-relief mechanisms for Ge/Si(100) coherent islands. Ge/Si(100) islands were grown at temperatures between 450 deg C and 650 deg C for effective Ge coverages between 3.5 and 14.0 monolayers. We find that the mean dome size increases and the onset of dislocation introduction is delayed with increasing growth temperature. Also, for temperatures greater that 600 deg C, very large hut clusters are observed which populate a peak in island size distributions distinct from and between those of huts and domes. For temperatures greater that 550 deg C, we find that large dome clusters may form trenches at their perimeter which may extend well into the Si substrate. Increasing growth temperature reduces the size at which these trenches appear. Cross-sectional energy dispersive x-ray nanoanalysis confirms that Si readily diffuses into the Ge clusters at temperatures greater than 600 deg C. This Si diffusion into the Ge clusters is responsible for the increase in dome size and delay of dislocation introduction with increasing growth temperature and the existance of very large hut clusters. A simple atomistic elastic model is presented which explains this complex alloying behavior. This model is also used to interpret the formation of trenches. We find that trench formation always lowers the total elastic energy of islands by removing material from the most highly strained regions of the island via surface diffusion.

11:15 AM I5.8
NUCLEATION VS. INSTABILITY PHENOMENA ON THE ENERGETIC PATHWAY OF SiGe/Si GROWTH.
Silke H. Christiansen, Michael Becker, Martin Albrecht and Horst P.Strunk, Universitaet Erlangen-Nuernberg, Institut fuer Werktstoffwissenschaften, Lehrstuhl Mikrocharakterisierung, Erlangen, GERMANY; H. Wawra, Institut fuer Kristallzuechtung, Berlin, GERMANY.

Using liquid phase epitaxy from Bi solution a growth technique that by its nature performs near thermodynamic equilibrium we analyse the morphological transition from two-dimensional growth via rippling to island formation in the model system SiGe/Si(001). We use both atomic force microscopy and transmission electron microscopy to analyse shape and size of the three dimensional morpholgies Systematic growth experiments as dependent on growth rate and temperature and misfit allowed to investigate the ripple concerning stable wavelength, wavelength fluctuations, and aspect ratios. Growth of a layer with thickness gradient allows to study the structural development of the layer with time from ripple via coexistence to an island stage at different coverages. From a matrix of that type of gradient specimens we determine nucleation energies of islands as dependent of the misfit. We show that the island nucleation process can be described in the classical framework of the Avrami-Johnson-Mehl model. Moreover we show that island formation essentially influences the amplitude and wavelength of the surrounding ripples. While ripples that surround an island are dissolved, the amplitude of ripples in a critical distance to the island increase and then decrease again with increasing distance to the island.

11:30 AM I5.9
IDENTIFICATION OF SHAPE TRANSITIONS IN COHERENT Ge/Si ISLANDS USING TRANSMISSION ELECTRON MICROSCOPY. Chuan-Pu Liu, William L. Henstrom, David G. Cahill, Univ. Illinois at U-C, Mat. Res. Lab., Urbana, IL; J. Murray Gibson, Mat. Sci. Div., Argonne National Laboratories, Argonne, IL.

As a consequence of strain relaxation, Ge coherent islands on Si(001) substrate evolve to different shape (aspect ratio) during deposition. By measuring the strain in an individual island within a population of islands using a simple and robust transmission electron microscopy-based technique, one can identify the island shape (aspect ratio) easily because island shape is a function of strain. We show that there is a metastable Ge island involved in the shape transition between pyramids and domes. The strain relaxation changes discontinuously as islands grow from pyramids to the metastable form and then again to domes indicating that the shape transition between pyramids and domes is first order. We also show that the shapes of this metastable island as well as pyramids and domes can be studied on both plan-view and cross-section samples. In-situ observation of strain(shape) evolution in Ge islands is also discussed.

SESSION I6/N7: JOINT SESSION: ATOMIC SCALE STUDIES
Chair: Venkatesh Narayanamurti
Wednesday Afternoon, December 1, 1999
Wellesley (M)

1:30 PM *I6.1/N7.1
ATOMIC-RESOLUTION Z-CONTRAST IMAGING AND ITS APPLICATIONS IN STUDIES OF ORDERED STRUCTURES.
S.J. Pennycook; Y. Yan, A. Norman, Y. Zhong, S.P. Ahrenkiel, M. Al-Jassim and A. Mascarenhas, National Renewable Energy Laboratory, Golden, CO.

In the last few years the scanning transmission electron microscope (STEM) has become capable of forming electron probes of atomic dimensions, as small as 0.13 nm in diameter. This has made possible a new approach to high-resolution electron microscopy, Z-contrast imaging. The Z-contrast image is an incoherent image, formed by mapping the intensity of high-angle scattered electrons as the probe is scanned across the specimen, and can be directly inverted to atomic structure. Because high angle scattering comes predominantly from the atomic nuclei, the scattering cross section depends on atomic number (Z) squared. The images therefore represent a direct map of the scattering power at atomic resolution. Z-contrast imaging is therefore an ideal technique to study compositional ordering at the atomic scale. In this presentation, examples are given of ordering in ferroelectric materials and III-V semiconductor alloys.
In ferroelectric materials, the atomic structure of ordered domains, both La-doped and undoped in $Pb(Mg_{1/3}Nb_{2/3})O_3$ is studied. The ordered domain structure in both cases is determined to be in agreement with the charge-balanced random-site model, and inconsistent with the space-charge model. It is shown that La doping in $Pb(Mg_{1/3}Nb_{2/3})O_3$ enhances not only the domain size but also the degree of ordering. In K-doped $PbZrO_3$, antiparallel cation displacements are observed but do not present any ordered structure. K is found to substitute for Pb uniformly in most ordered domains, while in some ordered domains, nonuniformly distributed K sites are also observed.
In III-V semiconductor alloys, spontaneous atomic ordering is

common. It has profound effects on the electrical and optical properties of the materials. To understand the details of the ordered structures is important to understand their properties. Ordered structures in $GaAs_ySb_{1-y}$ and $Ga_yIn_{1-y}P$ are presented. In $GaAs_ySb_{1-y}$, a new ordered structure is observed, containing a periodic array of antiphase domains with Cu-Au ordering of the As and Sb atoms on the {110} and {100} planes. The antiphase domain boundaries are along the [110] direction and spaced by $2d_{110}$ of the zinc-blende structure. In $Ga_y In_{1-y}P$, the ordered domains exhibit Cu-Pt ordering of As and P atoms. The ordered domains show two variants, [111] and $[\bar{1}\bar{1}1]$ arranged periodically to form an orientational superlattice resulting in a discontinuity of the angular momentum. The structures of the antiphase domain boundaries, the orientational domain boundary and the interface between two ordered variants are discussed.
*This research was sponsored by the Division of Materials Sciences, U. S. Department of Energy under contract No. DE-AC05-96OR22464 with Lockheed Martin Energy Research Corp.

2:00 PM *I6.2/N7.2
RAPID-QUENCH STM STUDIES OF InAs QUANTUM DOT FORMATION ON GaAs (001). P.B. Joyce, T.J. Krzyzewski, G.R. Bell, T.S. Jones, B.A. Joyce, Centre for Electronic Materials and Devices, Imperial College, London, UK.

The precise formation mechanism of InAs quantum dots (QDs) grown on As-rich GaAs(001)is still unknown, although the problem is of wide interest. Scanning tunneling microscopy (STM) provides a powerful probe of this process, particularly at the initial stages where three-dimensional features are very small. Our room temperature STM is attached directly to a molecular beam epitaxy chamber via a fast transfer system which allows the growth process to be interrupted and the sample quenched in less than ten seconds. Results from these STM studies on the initial formation of QDs will be presented along with structural data obtained by other methods such as reflection high energy electron diffraction (RHEED) and scanning transmission electron microscopy. For example, we have observed temperature-dependent alloying of nominally pure InAs QDs during both growth and capping. Other topics will include the relationship between QD shape and RHEED patterns, the atomic structures of the 'wetting layer' and QD facets, the differences between the (001) surface and other low index faces, and the effects of growth rate on the optical properties of QDs.

2:30 PM I6.3/N7.3
FORMATION MECHANISM OF METAL OXIDE QUANTUM DOTS: THEORETICAL SIMULATION STUDY. Momoji Kubo, Yusaku Inaba, Takayuki Onozu, Seiichi Takami, Akira Miyamoto, Tohoku Univ., Dept. of Materials Chemistry, JAPAN; Masashi Kawasaki, Tokyo Inst. of Technol., Interdisciplinary Graduate School of Eng., Yokohama, JAPAN; Mamoru Yoshimoto, Tokyo Inst. of Technol., Materials and Structures Lab., Yokohama, JAPAN; Hideomi Koinuma, Tokyo Inst. of Technol. and CREST-JST, Materials and Structures Lab., Yokohama, JAPAN.

Artificial construction of atomically defined metal oxide layers is important in making electronic, magnetic, and optical devices. More recently, the fabrication of metal oxide self-organized quantum dots on metal oxide substrates has gained much attention because of their interesting physical properties such as ultraviolet laser emission. It is experimentally well known that the formation of quantum dots is due to the large lattice mismatch beteen the substrate and thin film. This type of epitaxial growth is designated as higher-order epitaxy. The detailed understanding of the formation mechanism of self-organized quantum dots has been desired to control the size, shape, and crytallinity of the quantum dots. However, experimentally it is impossible to clarify the formation mechanism of the self-organized quantum dots on atomic scale. Hence, in the present study, we employed our crystal growth molecular dynamics simulator MOMODY [1-4] to simulate the formation process of various metal oxide quantum dots on sapphire(0001) surface. For example, when we continuously deposited MgO molecules on sapphire(0001) at 1000 K, the formation of MgO quantum dots was obserbed. The MgO quantum dots on sapphire(0001) has (111) orientaion and this formation process follows Stranski-Krastanov mode. Moreover, we suggested that the high flexibility of the coordination number of Al atoms on the topmost sapphire surface is a main reason for the higher order epitaxy and the formation of quantum dots. To the best of our knowledge, this is a first simulation study of the formation mechanism of self-organized quantum dots.
[1] M. Kubo, Y. Oumi R. Miura, A. Stirling, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and H. Koinuma, Phys. Rev. B 56 (1997) 13535.
[2] M. Kubo, Y. Oumi R. Miura, A. Stirling, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and H. Koinuma, J. Chem. Phys. 109 (1998) 8601.
[3] M. Kubo, Y. Oumi R. Miura, A. Stirling, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and H. Koinuma, J. Chem. Phys. 109 (1998) 9148.
[4] M. Kubo, Y. Oumi, H. Takaba, A. Chatterjee, and A. Miyamoto, J. Phys. Chem. B 103 (1999) 1876.

3:15 PM *I6.4/N7.4
FORMATION OF COHERENT α-Sn QUANTUM DOT ARRAYS VIA PHASE SEPARATION FROM HOMOGENEOUS ULTRATHIN Sn_xSi_{1-x}/Si AND Sn_xGe_{1-x}/Ge EPITAXIAL ALLOY FILMS. Harry A. Atwater, Kyu S. Min and Regina Ragan, Thomas J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, CA.

Diamond cubic α-Sn is a direct band gap semiconductor and band structure calculations also predict a direct and tunable energy gap composition range for the Sn_xSi_{1-x} and Sn_xGe_{1-x} alloy systems. One approach for realization of these compound semiconductors in the direct band gap range is synthesis of a self-ordered, coherently-strained Sn-rich quantum dot array via phase separation of chemically metastable epitaxial Sn_xSi_{1-x} and Sn_xGe_{1-x} alloys. We discuss a novel two-step process for α-Sn quantum dot synthesis within Si or Ge, where the enthalpy of mixing is highly positive. First, epitaxially stabilized homogeneous Sn_xSi_{1-x} and Sn_xGe_{1-x} metastable solid solutions are grown by temperature-modulated molecular beam epitaxy. The as-grown homogeneous film is then thermally annealed in high vacuum, whereupon the quantum dots precipitate as the ultrathin alloy film phase separates. The quantum dots appear in high-resolution transmission electron micrographs as square-shaped with facets along the $< 100 >$ direction, and the size ranges from 2 nm to 6 nm. The early stages of phase separation are consistent with a spinodal decomposition mechanism, and late-stage α-Sn dot evolution occurs via coarsening. Results of optical characterization, including infrared absorption and photoluminescence, will be related to the kinetics of phase separation.

3:45 PM *I6.5/N7.5
CHARACTERIZING ATOMIC-SCALE COMPOSITION VARIATIONS IN EPITAXIAL III-V MATERIALS WITH CROSS-SECTIONAL SCANNING TUNNELING MICROSCOPY Jeremy D. Steinshnider, John R. Harper, Michael B. Weimer, Texas A&M University, Dept of Physics, College Station, TX.

Many important issues in the epitaxial growth of III_a-V_c / III_b-V_d semiconductor heterostructures and III_a-III_b-V semiconductor alloys present a common theme from the standpoint of materials characterization: they require the real-space visualization of atomic-scale chemical heterogeneity together with a quantitative assessment of its influence on material quality. We illustrate how cross-sectional scanning tunneling microscopy (STM) can be used to address this theme by examining several fundamental material phenomena. We first demonstrate how anion cross incorporation and segregation may be distinguished from each other and quantitatively characterized through V_c-V_d site discrimination in AlSb/GaSb/InAs multiple quantum wells and GaInSb/InAs superlattices fabricated with molecular beam epitaxy. We next indicate how III_a-III_b site discrimination similarly facilitates a direct visualization of the cation sublattice order in GaInP alloys grown by metal-organic vapor phase epitaxy and show that the extent of this order is reflected on nanometer length scales by an appropriate pair correlation function constructed from the STM data. Finally, we describe how these apparently unrelated problems are connected with a discussion of interface bond identification in antimony-based heterostructures.
Work performed in collaboration with D. Zhang, C.-H. Lin, and S.S. Pei, University of Houston; G. Turner, MIT Lincoln Laboratory; D. Chow, HRL Laboratories; and M. Hanna, National Renewable Energy Laboratory, and supported in part by the National Science Foundation, Division of Materials Research, and the Air Force Research Laboratory.

4:15 PM I6.6/N7.6
MULTIMILLION ATOM SIMULATIONS OF ATOMIC-LEVEL SURFACE STRESSES AND MIGRATION PROCESSES ON InAs/GaAs MESAS. Xiaotao Su, Aiichiro Nakano, Sanjay Kodiyalam, Rajiv K. Kalia, Priya Vashishta, Concurrent Computing Laboratory for Materials Simulations, Dept. of Physics & Astronomy, Dept. of Computer Science, Louisiana State University, Baton Rouge, LA; Anupam Madhukar, University of Southern California, Los Angeles, CA.

Large scale molecular dynamics simulations are performed to investigate the atomic-level surface stresses and migration processes on InAs/GaAs mesas. The simulations are based on an interatomic-potential scheme for mixed InAs/GaAs systems which depends on the local chemical composition. Multiresolution techniques are used to speed up the simulations. InAs/GaAs square mesas with {103}-type side walls and InAs/GaAs stripe mesas with {113}-type side walls are studied. Results will be presented for surface atomic

stresses on the side walls with different monolayers of InAs, stress gradient on the side walls, and atomic-level distribution of hydrostatic pressure. Work supported by NSF, DOE, AFOSR, USC-LSU MURI, ARO, NASA, PRF, NSF USA-Japan International Grant, and LEQSF.

SESSION I7: POSTER SESSION:
ORDERING/COMPOSITION MODULATION /
3-D ISLANDING
Chairs: David M. Follstaedt and Angelo Mascarenhas
Wednesday Evening, December 1, 1999
8:00 P.M.
Exhibition Hall D (H)

I7.1
COMPOSITION AND THICKNESS EFFECTS ON ATOMIC ORDERING IN THE GALLIUM-INDIUM PHOSPHIDE EPITAXIAL LAYERS. Adi Goldner, Emil Zolotoyabko, Yigal Komem, Technion-IIT, Dept of Materials Engineering, Haifa, ISRAEL.

CuPt-B-type ordering in the $Ga_xIn_{1-x}P$ system has attracted a lot of attention due to its influence on the band gap. However, the mechanism of ordered phase stabilization within a film interior under in situ heat treatment, accompanying epitaxial growth and acting to destroy an ordered state, remains unclear. In this paper we investigated atomic ordering in the $Ga_xIn_{1-x}P$ layers ($0.47 < x < 0.54$) MOCVD grown on GaAs substrates and having thicknesses of 50, 100 and 1000 nm. Our research focused on the thickness-dependent features in the ordering phenomenon, bearing in mind that the layer thickness is linearly proportional to the duration of growth, and thus in thicker layers the heat effect should be more pronounced. Epitaxial layers of $Ga_xIn_{1-x}P$/GaAs were studied by transmission electron microscopy, high-resolution X-ray diffraction, and photoluminescence measurements. Special attention was paid to the precise determination of strain levels and compositions, because these data are used to extract the ordering degree η from photoluminescence spectra. High-resolution X-ray diffraction measurements with quasi-forbidden reflections allowed us to determine Ga concentration with an absolute precision of $\delta x = 0.0015$. As a result, we were able to derive the degree of ordering, $\eta(x)$, as a function of the layer composition, x, in the close vicinity of $x = 0.5$, which composition favors complete ordering, $\eta = 1$. The $\eta(x)$-dependencies exhibited bell-like shapes with parameters depending on the sample thickness. With increasing thickness, the bell-shaped $\eta(x)$-curves were found to be broadened, their maximum values to be reduced and the x-position of the η-maximum to be shifted from expected $x = 0.5$ to $x = x_m = 0.516$. The latter composition corresponds to the complete matching of the $Ga_xIn_{1-x}P$ and GaAs lattice parameters. A semi-phenomenological model is developed which explains experimental findings in terms of concentration fluctuations across the layer.

I7.2
CuPt-B ORDERED MICROSTRUCTURES IN GaInP AND GaInAs FILMS. S.P. Ahrenkiel, K.M. Jones, R.J. Matson, M.M. Al-Jassim, Y. Zhang, A. Mascarenhas, D.J. Friedman, D.J. Arent, J.M. Olson, M.C. Hanna, National Renewable Energy Laboratory, Golden, CO.

We examine CuPt-B atomic sublattice ordering in $Ga_{0.51}In_{0.49}P$ (GaInP) and $Ga_{0.47}In_{0.53}As$ (GaInAs) III-V alloy films grown by atmospheric- and low-pressure metalorganic chemical vapor deposition on singular and vicinal (001) substrates. The influences of growth conditions and substrate miscut on double- and single-variant ordered microstructures are investigated using transmission electron microscopy (TEM). Relatively thick (>1-2 μm) double-variant ordered GaInP and GaInAs films show complementary superdomain formation. Single-variant ordered films on <111>B-miscut substrates contain single-phase domains, separated by antiphase boundaries (APBs). The appearance of APBs in TEM dark-field images is anticipated from electron diffraction theory.

I7.3
SINGLE AND DOUBLE VARIANT CuPt-B ORDERED GaInAs. R.L. Forrest, R.T. Nielsen, M. S. Goorsky, Dept of Materials Science and Engineering, University of California, Los Angeles, CA; Y. Zhang, A. Mascarenhas, M. Hanna, NREL, Golden, CO.

Nominally lattice-matched GaInAs layers grown by metal organic vapor phase epitaxy on InP substrates have been studied using high-resolution x-ray diffraction (HRXRD) to determine the growth conditions under which ordering is introduced. HRXRD provides an independent means to quantify the order parameter of semiconductor heterostructures as well as the ordering on different {111} planes, i.e., double variant ordering. This independent means to determine ordering provides for a better understanding of the effects of ordering on the electronic and optical properties. In all cases, the epitaxial layers studied were closely lattice matched to the substrate, with strains less than or equal to 0.09%. Double variant ordering was determined to occur for epitaxial layers grown on exact (001) InP substrates, with an order parameter of about 0.1 in both variants. For substrates which were miscut by 6 degrees, only single variant ordering was detected. In these cases, an order parameter as high as 0.28 was measured for certain growth conditions. The layers grown on vicinal substrates are all of high crystalline quality, those on (001) substrates exhibit some mosaic spread.

I7.4
ELECTRONIC AND OPTICAL PROPERTIES OF MICRO ORDERED DOMAIM TWINS IN GaInP ALLOYS. Yong Zhang, B. Fluegel, S.P. Ahrenkiel, J.D. Perkins, D.J. Friedman, J.F. Geisz, J.M. Olson and A. Mascarenhas, National Renewable Energy Laboratory, Golden, CO.

It is known that CuPt ordering occurs only in the two [111]B directions in GaInP alloys. When the GaInP epilayer is grown on an exact (001) or [111]A tilt GaAs substrate, the two ordered variants are equally favorable and so, ordered domain twins appear in ordered GaInP epilayers grown on such substrates. The sizes of the periodically alternating domain twins are small enough to cause such structures to behave as orientational superlattices.[1] The electronic and optical properties of such superlattices are qualitatively different from single-variant CuPt ordered structures. We will present a comparative study between single-variant ordered samples and double-variant ordered samples with micro domain twins,[2] using techniques such as TEM, photoluminescence, photoluminescence excitation, time-resolved pump-probe and electroreflectance. The experimental results clearly demonstrate the electronic properties of orientational superlattices. [1] A. Mascarenhas et al, Solid State Commun. 100, 47 (1996); Yong Zhang and A. Mascarenhas, Phys. Rev. B55, 13100 (1997). [2] Yong Zhang et al, Solid State Commun. 109, 99 (1998).

I7.5
LOCAL ORDER OF Te IMPURITY ATOMS IN HEAVILY DOPED GaAs:Te AND ACCOMPANYING ELECTRON LOCALISATION EFFECT. T. Slupinski[a], E. Zielinska-Rohozinska, Inst. of Experimental Physics, Warsaw University, Warsaw, POLAND; [a] present address: Kanagawa Acad. of Science and Technology, Kawasaki, JAPAN.

In this presentation we show the results of joined extended studies of the free electron concentration and X-ray diffuse scattering (detected by HR XRD - reciprocal space maps) as a function of Te atoms concentration in GaAs and controlled annealing of samples at high temperatures 700—1200 °C. Main results are:
1) In GaAs samples with Te concentration higher than about $Te = 4 \cdot 10^{18}$ cm^{-3} the free electron concentration can be reversible changed between low value ($n < Te$ and high one $n \approx Te$ merely by a proper annealing,
2) Strong X-ray diffuse scattering is observed in annealed samples, if electron concentration is lowered. Intensity of this scattering is in a perfect coincidence with the changes of the electron concentration caused by the annealing,
3) The diffuse scattering observed comes from the crystal lattice distortions, as it is concluded from X-ray scattering in the vicinity of quasi-forbidden reflections,
4) Detailed features of X-ray scattering in the reciprocal space can be very well understood within Krivoglaz microscopic model (1959) of scattering due to local correlations of impurity positions (locally the creation of impurity—impurity pairs) in a solid solution (local order) and related crystal lattice distortions. This old model has never been used in the literature to an analysis of scattering results in semiconductors, according to our knowledge,
5) Electron localisation can be quantitatively understood assuming that the creation of the impurity—impurity pair is governed by the electron energy (Fermi level) in GaAs at high temperature.
Model of the structure of GaAs:Te solid solution with local order will be outlined, as it emerges from X-ray studies. Our results indicate that due to an evidence of structural changes of critical character and an arrising of long range fluctuations accompanying electron localisation caused by the annealing of heavily doped n-GaAs the solid solution of donor impurities in GaAs exhibits features of a structural phase transition. These results are important for an understanding of known limits of the free electron concentration in heavily doped n-GaAs. Also they support the hypothesis of an existence of chemically bonded dimers of impurity atoms, formulated during last years in the literature and propose electron energy dependent mechanism of their creation.

I7.6
A-TYPE ORDERING IN $Al_{0.5}In_{0.5}As$ GROWN BY METALORGANIC-VAPOR-PHASE EPITAXY. Tohru Suzuki, Opto-Electronics & High-Frequency Device Res. Labs., NEC Corp., Toshinari Ichihashi, Fundamental Res. Labs., NEC Corp., Masayoshi

Tsuji, Opto-Electronics & High-Frequency Device Res. Labs., NEC Corp., Tsukuba, JAPAN.

Triple-Period-A(TP-A) and CuPt-A type ordering as well as conventional CuPt-B type ordering have been observed in III-V semiconductor alloys grown on (001) III-V substrates by molecular beam epitaxy (MBE). Surface reconstructions during growth in which these types of ordering are formed are (2x3), (1x2) and (2x1), respectively. These relations definitively established the responsibility of surface re-constructions during growth to ordering on a sublattice. In turn, frequent observations of CuPt-B type ordering in metalorganic-vapor-phase-epitaxially (MOVPE) grown III-V semiconductor alloys indicate the existence of (2x1) reconstruction during these MOVPE growths. This leads to the question whether A-type ordering such as TP-A and CuPt-A can be formed in MOVPE grown III-V alloys as in MBE grown alloys. We report for the first time observation of TP-A and CuPt-A type ordering in $Al_{0.5}In_{0.5}As$ grown by MOVPE at a low temperature of 500 degree C. This indicates that arsenic double layer structures of (2x3) and (1x2) exist in this alloy during growth even in MOVPE when growth temperatures are low.

I7.7
USE OF MISCUT SUBSTRATES TO EXTEND LATERAL COMPOSITION MODULATIONS IN InAs/AlAs SUPERLATTICES. John L. Reno, David M. Follstaedt, Stephen R. Lee and Eric D. Jones, Sandia National Laboratories, Albuquerque, NM; Andrew G. Norman, Scott P. Ahrenkiel, Helio R. Moutinho and Angelo Mascarenhas, National Renewable Energy Laboratory, Golden, CO.

The microstructure of composition modulation in $(InAs)_n/(AlAs)_m$ short-period superlattices grown on (001) InP has been well characterized. For optimum growth conditions (n $\approx$ m = 0.5 - 2.0, $T_{gr} \approx 530°C$), the laterally modulated regions grow as vertical columns with only short extension in the growth plane (≈ 0.1 μm). Moreover, the lateral modulation occurs equally along two directions in the growth plane; for superlattices grown with moderate average tensile strain (< 0.4% in-plane strain), these are [130] and [310]. We have also found that the composition variations produced in these alloys are quite large: local enrichments in In concentration up to $In_{0.76}Al_{0.24}As$ have been determined. With the intent of producing extended modulations in the growth plane that are along one direction only, we are examining growth on miscut substrates. We have grown superlattices with n,m $\approx$ 2 and moderate tensile strain on oriented substrates, as well as substrates miscut 2° towards four different directions. The different miscut orientations vary in their relationships to the prefered [130] and [310] modulation directions of the oriented samples. TEM, AFM and x-ray diffraction indicate that strong modulation is present in all the specimens, but for miscuts toward (101), the modulation has one predominate direction. Furthermore, the modulated segments are longer, extending 0.2 - 0.4 μm in the growth plane. Thus growth on miscut substrates is producing more nearly ideal modulation geometries and microstructures for studies of electronic properties. Our results suggest that surface steps may play an important role in determining the in-plane organization of modulated regions. Properly miscut surfaces may lead to modulated structures that confine carriers to a single set of InAs-rich planar regions.

I7.8
PROFILING COMPOSITION VARIATIONS IN COMPOSITION-MODULATED GaP/InP SHORT-PERIOD SUPERLATTICES USING RESONANCE RAMAN SCATTERING. Hyeonsik M. Cheong, Yong Zhang, A.G. Norman, J.D. Perkins and A. Mascarenhas, National Renewable Energy Laboratory, Golden, CO; K.Y. Cheng and K.C. Hsieh Dept. of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Urbana, IL.

We use Resonance Raman scattering and electroreflection measurements to profile the the composition and strain variations in laterally composition modulated GaP/InP short-period superlattices. The electroreflectance spectra of a $GaP_{2.2}/InP_{2.0}$ short-period superlattice give the fundamental band-gap energy of the lateral superlattice at 1.69±0.05eV, which is about 210 meV lower than the band gap energy of a GaInP random alloy with the same overall composition. The resonance Raman scattering measurements reveal strong dependences of the phonon spectrum on the polarization and the excitation energy. In resonance Raman spectra measured with the polarization of both excitation and scattered photons along the composition modulation direction, the GaP-like longitudinal optical (LO) phonon redshifts by 4.0±0.5 cm^{-1} near the resonance with the fundamental energy gap. On the other hand, when the polarizations are orthogonal to the composition modulation, the LO phonons redshift as much as 16 cm^{-1} at low excitation energies. A comparison of the experimental data with a model calculation gives the average In composition in the In-rich region as 0.70±0.02, and the average Ga composition in the Ga-rich region as 0.68±0.02. Our result also indicates that there are small volumes (less than 1% volume fraction) with very high In mole fraction.

I7.9
RECIPROCAL SPACE X-RAY MAPPING AND TRANSMISSION ELECTRON MICROSCOPIC STUDIES OF COINCIDED δ-InAs AND As-CLUSTER SUPERLATTICES IN GaAs FILMS GROWN BY MOLECULAR-BEAM EPITAXY AT LOW TEMPERATURE. V.V.Chaldyshev, N.A. Bert, N.N. Faleev, Yu.G. Musikhin, A.E. Kunitsyn, A.F.Ioffe Physical-Technical Institute, St. Petersburg, RUSSIA; V.V. Preobrazhenskii, M.A. Putyato, B.R. Semyagin, Institute of Semiconductor Physics, Novosibirsk, RUSSIA; P. Werner, Max-Planck-Institute of Microstructure Physics, Halle, GERMANY; Y. Takeda, Nagoya University, Nagoya, JAPAN.

During the last few years nanoscale objects in GaAs matrix have attracted much attention due to interesting electronic and optical properties. These objects can be produced either on the growth surface using Stranski-Krastanow mechanism or in the film bulk due to precipitation a supersaturated solid solution. The latter case can be realized by low-temperature (LT) molecular-beam epitaxy (MBE) when a very high arsenic excess is incorporated into the growing film. The post-growth annealing leads to formation of nanoscale arsenic clusters built in GaAs matrix. In conventional LT GaAs the spatial cluster distribution is random, however thin InAs insertions cause formation of two-dimensional cluster sheets. In this paper we perform LT MBE and subsequent anneal of InAs/GaAs superlattices with the InAs layers as thin as 1 monolayer or less. Reciprocal space x-ray mapping and transmission electron microscopy are employed to assess the crystalline quality and parameters of both InAs and As-cluster superlattices. The as-grown InAs/GaAs superlattices were found to be very perfect in spite of the high (10^{20} cm^{-3}) concentration of excess-arsenic-related point defects. Formation of two-dimensional cluster sheets at InAs layers upon annealing was accompanied by smoothing of InAs/GaAs interfaces, however the cluster system does not produce any noticeable x-ray diffuse scattering. The growth and annealing conditions were found which provided accumulation of the great majority of the clusters in a multiperiodic regular superlattice.

I7.10
SELF-ORGANIZED MICROSTRUCTURES IN EPITAXIAL ANTIMONIDE ALLOYS. K. Rajan, Y-C. Chen, V. Bucklen, Rensselaer Polytechnic Institute, Troy, NY; C. Wang, Lincoln Laboratories, Lexington, MA; G. Charache, G. Nichols and P. Sanders, Lockheed-Martin, Schenectady, NY.

In this paper we provide a detailed diffraction / imaging study of the development of periodic self- organized structures within single layer epitaxial InGaAsSb/ GaSb heterostructures. The influence of surface crystallography and alloy composition have been studied . Apart from transmission electron microscopy imaging studies, we have conducted high resolution X-ray diffraction and uniquely coupled that with electron diffraction rocking curves to study the details of the phase instabilities associated with growth parameters in this quaternary alloy system. The results are interpreted in terms of fundamental mechanisms associated with ordering and spinodal decomposition

I7.11
THERMODYNAMIC STABILITY OF LATERALLY COMPOSITION-MODULATED PHASES IN ULTRATHIN SURFACE ALLOY FILMS. Vidvuds Ozolins, Mark Asta, J.J. Hoyt, Sandia National Laboratories, Computational Materials Science Dept, Livermore, CA.

Ordering and clustering instabilities in alloys are typically governed by the Fourier transform of the effective pair interactions, $V(\mathbf{k})$. In pseudomorphic ultrathin surface alloys $V(\mathbf{k})$ is proportional to $-k$ at the origin, thereby guaranteeing a minimum at $\mathbf{k} \neq 0$. As a consequence, disordered alloy films below a certain critical temperature always exhibit *ordering* instabilities with respect to long-period composition waves. These instabilities lead to ordered phases, similar to the ones observed in lateral composition modulation in semiconductors and long-period stripe and droplet phases in metal alloy films.

I7.12
TEM INVESTIGATION OF SELF-ORGANIZED PbSe QUANTUM DOTS AS A FUNCTION OF SPACER LAYER THICKNESS AND GROWTH TEMPERATURE. H.H. Kang, L. Salamanca-Riba, Materials and Nuclear Engineering Department, University of Maryland, College Park, MD; M. Pinczolits, G Springholz, G. Bauer, Institut für Halbleiterphysik, University of Linz, Altenbergerstr, Linz, AUSTRIA.

The study of the morphology, lateral, and vertical correlation of self-organized PbSe quantum dots in PbEuTe is presented. The samples consist of quantum dot superlattices of n periods of

(PbSe/PbEuTe) grown on PbTe/(111)BaF_2 by the S-K mode using MBE. The PbEuTe spacer thickness was varied from 32.4 nm to 312 nm and the growth temperature was varied between 335°C and 380°C. Our TEM and x-ray results show very good lateral and vertical correlation of the dots. The dots form an array with either an a/b/c/a/b/c/... or a/a/a/... vertical stacking sequence along the [111] growth direction. The stacking sequence is strongly controlled by the thickness of the PbEuTe spacer layer and the growth temperature. The best a/b/c/... spatial correlation was obtained for temperatures around 380°C and spacer thickness of ~40 nm. The dots are highly strained and form triangular pyramids with (111) bases and (100) facets as observed by AFM. And the shape of dots also varies with changing the PbEuTe spacer thickness. An analysis of the spatial correlation of the dots, the size and shape of the dots and their composition will be presented.

I7.13
TRANSMISSION ELECTRON MICROSCOPY INVESTIGATION OF THE MORPHOLOGY AND THE COMPOSITION OF $In_xGa_{1-x}As/GaAs$ QUANTUM DOTS. Xiaozhou Liao, Jin Zou, David J.H. Cockayne, The University of Sydney, Australian Key Centre for Microscopy and Microanalysis, Sydney, NSW, AUSTRALIA; Rosa Leon, California Institute of Technology, Jet Propulsion Laboratory, Pasadena, CA; Charlene Lobo, Australian National University, Department of Electronic Materials Engineering, Canberra, ACT, AUSTRALIA.

Unburied and buried $In_xGa_{1-x}As/GaAs$ quantum dots (QDs) have been investigated using transmission electron microscopy. The side projections of the surface profile of the unburied QDs obtained from a continuous tilting experiment of cross-section specimens are all arc shaped with constant base projections, which unambiguously show that the unburied dots are lens shaped with circular bases. Significant differences in the image features of the unburied QDs grown on (001) and vicinal (001) GaAs were seen in [001] on-zone bright-field images. Simulated images were obtained by modeling the strain field distribution of the QDs with finite element analysis and then using this model in dynamical electron diffraction contrast simulations. Comparison of the experimental images and the simulated images shows that: (i) indium segregates in the QDs, and (ii) the average indium content of the QDs is higher than the average indium content of the film. Cross-section $< 110 >$ images of buried QDs also suggests a lens shaped morphology, while the [001] on-zone bright-field images show a square contrast that suggests a QD morphology with four edges parallel to $< 100 >$. The simulated image, however, suggests that a buried lens shaped QD with a circular base can produce a square-shaped image. These observations lead to the conclusion that the buried QDs are also lens shaped.

I7.14
STRUCTURE OF InAs INCLUSIONS IN Si MATRIX. Nikolai. D. Zakharov, Peter Werner, Max-Planck Institute of Microstructure Physics, Halle/Saale, GERMANY; Robert Heitz, Dieter Bimber, Technical University of Berlin, GERMANY; Nikolai N. Ledentsov, Victor M. Ustinov, Dmitri V. Denisov, Boris V. Volovik, Zhores I. Alferov, A.F. Ioffe Physico-Technical Institute, St. Petersburg, RUSSIA; George E. Cirlin, Institute for Analytical Instrumentation, St. Petersburg, RUSSIA.

The importance of developing a technology that would allow optical and electronic devices to be easily and inexpensively integrated on a silicon wafer has been recognized. Such an advance would have a significant impact on display, communications and computer technologies. InAs inclusions embedded in Si matrix were grown by MBE under different conditions (substrate temperature, thickness of Si cap layer, annealing temperature). Some of the samples show a peak of photoluminescence with wavelength 1.3 m (0.95 eV). The appearance of this peak is interpreted in terms of a real crystal structure. HRTEM investigation shows the presence of small coherent InAs inclusions of about 3-4 nm in diameter. The computer simulations of the image contrast have been carried out revealing the InAs nature of observed clusters. In one of the specimens characterized by a relatively high photoluminescence efficiency a new type of InAs inclusions was found. They are defect free, have zigzag shape with periodicity of 1.5 nm and a size close to 10x5x1.3 nm. The absence of misfit dislocations indicates that they are coherently fit to the Si matrix and that their volume is well below the critical one.

I7.15
EVOLUTION OF THE SHAPE AND SIZE OF InGaAs SELF-ORGANIZED QUANTUM DOTS. Qianghua Xie, Semiconductor Research Center, Wright State University, Dayton, OH; J.L. Brown, R.L. Jones, J.E. Van Nostrand, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH.

A shape transformation of InGaAs self-organized quantum dots (QDs) formed via a fractional-monolayer deposition technique will be discussed first. At the initial stage, QDs are found to align along the valleys of an array of $[\bar{1}10]$ oriented multi layer mounds on the GaAs (001) surface. The density of QD increases rapidly from ~$110/\mu m^2$ (at a total deposition of 4 ML deposition) to ~$270/\mu m^2$ (at 5 ML) and saturates at this level upto 10 ML deposition. After the initial preferential nucleation along the valleys, QDs start to form on the mounds leading to a wider spread in lateral size and height. With further growth (at 7 ML), bi-modal QD height (peaked at 8.5 nm and 14.5 nm) and aspect ratio distributions sets in. Such bi-modal height and aspect ratio distributions directly confirm that the QDs transform from a shallower to a steeper shape as the volumes grow. Finally, the lateral size, height and aspect ratio all become convergent as a result of a *simultaneous* QD size equalization and shape stabilization. The QD size and shape evolution is also substantiated by the low temperature (4 K) photoluminescence (PL) data taken from samples with QDs capped by GaAs.

I7.16
THERMAL INDUCED FORMATION OF SILICON ISLANDS FROM SILICON ON OXIDE SUBSTRATES. Bernard Legrand, Vincent Agache, Vincent Senez, Didier Stievenard, IEMN, Villeneuve d'Ascq, FRANCE.

Starting from SOI substrates with 3 to 20 nm thick silicon layers, we show that silicon islands are created after a thermal heating in UHV in the 850-975°C range for a few minutes. The temperature formation of the islands increases with the silicon layer thickness and decreases when the native silicon oxide (1 nm) is previously removed with HF treatment. The island size (in a few 10 nm range) and their density ($\sim 10^9 cm^{-2}$) are measured with an atomic force microscope (AFM). This size can be reduced by thermal treatment (975°C,1 h). The island formation is monitored by using Auger spectroscopy. Finally, taking into account the stress variation versus temperature between silicon and silicon dioxide, a modelisation of the dot formation is tentatively proposed.

I7.17
NANO-STRUCTURAL INVESTIGATION OF InAs QUANTUM DOTS MULTI-STACKED ON GaAs (100) SUBSTRATES. Cheong Hyun Roh, Seon Woo Lee, Kwang Bo Shim, Hanyang Univ, Ceramic Processing Research Center, Dept of Ceramic Engineering, Seoul, KOREA; Young Ju Park, Kwang Moo Kim, Young Min Park, Eun Kyu Kim, Korea Institute of Science and Technology, Semiconductor Materials Laboratory, Seoul, KOREA.

InAs self-assembled quantum dots (SAQDs) were grown on a GaAs (100) substrate using the molecular beam epitaxy (MBE) technique. The InAs QDs were multi-stacked in various layer structures with 1, 3, 6, 10, 15 and 20 layers. The thicknesses of the GaAs spacer and the InAs wetting layer were 5.7 nm and 1.96 MLs, respectively. The nanostructural feature of the QD multi-stacking layers was characterized by scanning transmission electron microscopy (STEM) and photoluminescence (PL). According to STEM analysis, the quantum dots in the 6 stacking layer structure showed a good vertical alignment without defect generation, whereas volcano-like defects were vertically formed along the growth direction of QDs in the InAs stacking layers greater than 10 periods. Especially, in the cases of InAs stacking layers with 10 and 15 periods, the vertically columned InAs QDs grew in parallel with the growth direction of the volcano-like defects. The highest PL intensity was obtained from the specimen with 6 stacking layers and the energy of the PL peak was split with increasing stacking layer. The origin of the splitting phenomenon was estimated by the temperature-dependent PL measurement.

I7.18
THE GROWTH OF InAs SELF-ASSEMBLED QUANTUM DOTS ON InGaAs/InP BY METALORGANIC CHEMICAL VAPOR DEPOSITION. Hyouk Kwon, Sukho Yoon, Tae-Wan Lee, Youngboo Moon, Heedon Hwang and Euijoon Yoon, School of Materials Science and Engineering and Inter-university Semiconductor Research Center, Seoul National University, Seoul, KOREA; Young Dong Kim, Department of Physics, Kyung Hee University, Seoul, KOREA; Hyeonsik Michael Cheong, Solid State Spectroscopy Group, National Renewable Energy Laboratory, Golden, CO.

It is expected that the low-dimensional structures such as self-assembled quantum dot (SAQD) are necessary for the realization of next-generation, high-performance optoelectronic devices. Various dot/substrate combinations such as (In,Ga)As/GaAs, InP/InGaP/GaAs, InAs/In(Ga,Al)As/InP, and InAs/InP have been explored. Among these, the InAs/In(Ga,Al)As/InP system is very attractive for optical communication and environmental applications, since its emission wavelengths can be tailored to be larger than 1.3 μm. Nevertheless, quite a few reports have been made on the growth of InAs/InGaAs/InP quantum dots by molecular beam epitaxy (MBE), however, to the best of our knowledge, no reports have been

made for the growth of InAs/InGaAs/InP quantum dots by metalorganic chemical vapor deposition (MOCVD). We studied the growth of InAs SAQDs on InGaAs buffer layers lattice-matched to InP by MOCVD at various conditions. The InAs coverage, growth temperature and V/III ratio were varied, and the statistical information on the size distribution and the shape of SAQDs was obtained from atomic force microscopy (AFM). Some of the dots were capped with InGaAs with or without growth interruption, and their optical properties were studied by photoluminescence (PL). The average lateral dimensions of uncapped InAs SAQDs ranged from 75 to 95 nm, whereas the average heights ranged from 4.5 to 6.5 nm. We obtained high-density (2.2×10^{10} cm^{-2}) InAs SAQDs with fairly uniform size distribution (77±10 nm) at a growth condition of InAs coverage of 3.3 ML, growth temperature of 550°C, and V/III of 30. An intense PL peak at 1.89 μm (full-width at half-maximum of 46 meV) was observed at 8K from the sample capped with InGaAs after a 30-sec growth interruption in AsH_3 atmosphere, suggesting that the high-quality InAs/InGaAs SAQDs were obtained by MOCVD. Detailed information of the PL characteristics at various temperatures and pump powers will be presented.

I7.19
THEORETICAL STUDY ON THE EFFECT OF MISFIT DISLOCATIONS ON THE FORMATION OF InAs QUANTUM DOTS ON GaAs SUBSTRATES. Norihisa Oyama, Eiji Ohta, Keio Univ., Dept. of Applied Physics and Phisico-Informatics, Yokohama, Kanagawa, JAPAN; Ko Okajima, Kyozaburo Takeda, Dept. of Material Science and Engineering, Waseda Univ., Shinjuku, Tokyo, JAPAN; Kenji Shiraishi, Hiroshi Yamaguchi, NTT Basic Research Lab., Atsugi, Kanagawa, JAPAN; Tomonori Ito, NTT Photonics Lab., Atsugi, Kanagawa, JAPAN; Takahisa Ohno, National Research Institute for Metals, Tsukuba, Ibaraki, JAPAN.

It has been reported that the growth mode of InAs/GaAs strongly depends on the substrate orientations[1,2]. On a GaAs(001) substrate, the growth mode of InAs epilayers is Stranski-Krastanov type with the formation of self-organized quantum dots. On GaAs(110) and (111)A substrates, on the other hand, growth mode is two-dimensional and misfit dislocations are generated at the interfaces. In this study, we focused on the misfit dislocations at the InAs/GaAs heterointerfaces and clarified the microscopic origin of the dependence of the growth mode on the orientation. We investigated the microscopic structures of misfit dislocations generated at the InAs/GaAs(110) heterointerface by using the first-principles calculations. We found that the dislocation core has asymmetric five-fold coordinated In atoms. Such star-shaped dislocations have been previously unobserved in pure crystal. Because this core structure does not contain unfavorable bonds (As-As and Ga-Ga bonds), it is easy to generate the star-shaped dislocations during the initial stage of epitaxy. Accordingly, the growth mode of an InAs epilayer becomes two-dimensional after star-shaped dislocations are generated. This type of dislocation is also possible at InAs/GaAs(111)A interfaces from the geometrical viewpoint. Therefore, it is plausible that the growth mode on a (111)A substrate is also two-dimensional. On the other hand, star-shaped dislocations are impossible at InAs/GaAs(001) interfaces due to the geometry. On this substrate, the core structure of the misfit dislocations contains a 5- and 7-membered rings structure with unfavorable bonds (5-7 dislocations). Because the generation of 5-7 dislocations is restricted by the unfavorable structure, the growth mode on the (001) substrate becomes Stranski-Krastanov type with the formation of self-organized quantum dots. Consequently, our finding leads to the guiding principle that InAs quantum dots can be formed only when the generation of star-shaped dislocations is impossible. [1] J. G. Belk et al. , Phys. Rev. Lett. 78, 475(1997). [2] H. Yamaguchi et al., Phys. Rev. B55, 1337(1997).

I7.20
SELF-ORGANIZATION, SHAPE TRANSITION AND STABILITY OF EPITAXIALLY STRAINED ISLANDS. Y.W. Zhang, IMRE, National University of Singapore, SINGAPORE.

Strain-induced self-organization of epitaxial islands has drawn considerable attention due to potential application in the fabrication of optoelectronic and microelectronic devices. However there are many controversial issues that exist in the growth of epitaxially strained islands. In order to clear up the controversies, three-dimensional computer simulations are carried out to investigate the self-organization, shape transition and stability of epitaxially strained islands during controlled annealing. In the simulations, the strain energy density, surface energy density and surface energy anisotropy are taken into account. It is found that the phenomena of ripening or non-ripening, strong self-organization or weak self-organization, and shape transition or non-shape transition of the island arrays can be obtained by slightly changing the surface energy anisotropy. By linking the surface energy anisotropy to the change of the annealing temperature and the change of the materials compositions, the inconsistencies that exist in the experiments can be explained. Moreover, the present simulations predict that if we can choose the surface energy anisotropy by tailoring the materials composition and/or by changing the annealing temperature, then the strongly self-organized and non-ripening island arrays can be obtained.

I7.21
STRAINS IN SELF-ASSEMBLED InAs QUANTUM DOTS IN GaAs: A FINITE ELEMENT STUDY. G. Muralidharan, Institute of Microelectronics, Singapore, SINGAPORE.

One exciting area of semiconductor physics is the use of structures of low dimensions such as quantum dots obtained by self-organized growth. The self-organized growth is driven by the lattice mismatch strains between the material comprising the quantum dot structure and the substrate. One of the systems that have been studied widely is the InAs/GaAs system. InAs contained in a 1.7 monolayer InAs wetting layer on a GaAs substrate is known to aggregate into quantum dots due to a 7% lattice mismatch between InAs and GaAs. Further, vertically self-aligned quantum dots are known to occur when the InAs dots are embedded further in additional layers of GaAs. It is also well known that these quantum dots are lens-shaped when embedded in GaAs. Although the effect of coherency strains in causing self-alignment is very well recognized, the influence of the shape of these dots has received much less attention. Most theoretical calculations assume a pyramidal shape for these quantum dots to calculate strains induced by the presence of the layer. The present work is aimed at understanding the effect of the shape of the quantum dots on the strains induced in the substrate, the dot and the cap layer. Modeling has been accomplished by using the finite element method and a thermo-mechanical formulation of the problem. The effect of surface relaxation and implications for experimental measurements of such strains will also be illustrated in the calculations. The results of the simulation will be compared with the data available on the experimental measurements of strains.

I7.22
THEORETICAL STUDY ON MISFIT DISLOCATIONS IN SELF-ASSEMBLED GaSb QUANTUM DOTS ON GaAs(001) SURFACES. Ko Okajima, Kyozaburo Takeda, Dept. of Materials Science and Engineering, Waseda Univ., Shinjyuku, JAPAN; Norihisa Oyama, Eiji Ohta, Dept. of Applied Physics and Phisico-Informatics, Keio Univ., Yokohama, JAPAN; Kenji Shiraishi, NTT Basic Research Laboratories, Atsugi, JAPAN; Tomonori Ito, NTT Photonics Laboratories, Atsugi, JAPAN; Takahisa Ohno, National Research Institute for Metals, Tsukuba, JAPAN.

It has been reported that the GaSb self-assembled quantum dots on GaAs (001) substrates are formed during the initial heteroepitaxial stages with well-defined misfit dislocations. During GaSb deposition, the interface misfit-driven mechanism changes the epitaxy growth-mode from strain-induced 3D nucleation including spontaneous ordering of the misfit dislocations to 2D epitaxy. To gain a systematic understanding of this system, we calculated the free energy phenomenologically. The effects of the dislocation formation, surface energy, and island formation were included by parameterization in our calculations. The results show that the characteristic change in the dominant growth-mode in this system is mainly caused by the formation of misfit dislocations, which strongly relax the strain energy at the GaSb/GaAs(001) heterointerface. Because the parameter of the dislocation formation should be determined from the microscopic viewpoint, we investigated these misfit dislocations microscopically by using first-principles calculations. Using first-principle geometrical optimization, we found a 5&7 membered ring (MR) structure at the dislocation core. This structure was formed by the elongated cation-cation (Ga-Ga) or anion-anion (As-As) weak bonds. These weak bonds appeared on both Ga- and As-terminated surfaces, resulting in the formation of similar 5&7 MR structures on both surfaces. We also investigated square arrays of misfit dislocations generated at this interface; these results were compared with those of the InAs/GaAs (001) system.

I7.23
STRUCTURAL AND OPTICAL PROPERTIES OF SELF-ORGANIZED QDS IN InAs/$In_{0.53}Ga_{0.47}As$ MULTILAYERS ON (001)InP GROWN BY MOLECULAR BEAM EPITAXY. Zhong-zhe Sun, Ju Wu, Feng-qi Liu, Yong-hai Chen, Xiao-ling Ye, Wei-hong Jiang, Yue-fa Li, Bo Xu, Ji-ben Liang, Zhan-guo Wang, Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences. Beijing, PR CHINA.

In this work, we reported the self-organized InAs/$In_{0.53}Ga_{0.47}As$ QD multilayer grown on InP(001). A 5-period InAs quantum dots multilayer on InP substrate was demonstrated for the first time. The samples were grown by a Riber 32P MBE system; After oxide desorption, deposition of a 0.2μm $In_{0.53}Ga_{0.47}As$ buffer layer was followed by the growth of 5 bilayers, in which InAs QD layer with

certain nominal thickness were separated by 10nm $In_{0.53}Ga_{0.47}As$ spacer layer. The effective thickness of InAs was 1.9nm in the present work. The structure was terminated by a 70nm $In_{0.53}Ga_{0.47}As$ cap layer. Growth interruptions of 20s were used at both InGaAs/InAs heterointerfaces. The growth rates of InGaAs and InAs are ~0.76 and ~$0.41\mu m/h$, respectively; Arsenic vapor pressure used in growth was approximately $(8\tilde{}9) \times 10^{-6}$ Torr and the growth temperature was $510°C$.
The structural and optical properties were characterized using cross-sectional TEM and PL, respectively; In the TEM image, the coherent dots formation was evident through the characteristic dark/bright contrast related to different material composition. It was estimated that the average height and lateral size of dots was 3.6 and 21nm, respectively, and the ratio of height to lateral size was between 0.15~0.2. In PL measurement, narrow luminescence with FWHM of 26meV was achieved from QDs multilayer structure, which shows the potential for further optoelectronic application.

I7.24
SURFACE PHOTOABSORPTION MONITORING OF InAs/InP QUANTUM DOT FORMATION. Sukho Yoon, Heedon Hwang, Tae-Wan Lee, Youngboo Moon, and Euijoon Yoon, School of Materials Science and Engineering, Seoul National University, Seoul, KOREA; Young Dong Kim, Department of Physics, Kyung Hee University, Seoul, KOREA; Uk Hyun Lee and Donghan Lee, Department of Physics, Chungnam National University, Taejon, KOREA.

The self-assembled quantum dot (SAQD) formation has attracted a lot of attention for potential applications to high-performance electronic and optical devices. In molecular beam epitaxy systems, reflection high-energy electron diffraction has been used to monitor the 2D-3D transition. However, the high-pressure environment of metalorganic chemical vapor deposition (MOCVD) precludes the use of such a tool. Instead, optical techniques such as reflectance difference spectroscopy and spectroscopic ellipsometry have been used to investigate the initial stage of dot formation by MOCVD. In this paper, we present an *in situ* surface photoabsorption (SPA) study of the InAs quantum dot formation during growth interruption (GI) at different atmospheres. 2-monolayer-thick InAs layers were grown at 550°C on InP by MOCVD, and subsequently the 30-sec GI was provided at different atmospheres of AsH_3, PH_3 and H_2 before the InP capping layer growth. The SPA signal was recorded throughout the entire process. It increased linearly during the InAs growth, implying the two-dimensional InAs growth for all samples. The two-dimensional nature of InAs growth was confirmed by photoluminescence and transmission electron microscopy analysis of the capped samples without GI. During the GI at AsH_3 atmosphere, the SPA signal increased initially and then saturated. It did not changed at H_2 atmosphere and it, on the contrary, slightly decreased at PH_3 atmosphere. The samples with GI at AsH_3 atmosphere showed a QD photoluminescence (PL) peak at 0.77 eV, whereas those of the H_2- and PH_3-treated samples showed only PL peaks from thick InAs quantum wells with monolayer thickness fluctuation, judging from the energy level calculation of the biaxially strained InAs quantum wells. It was found that the GI atmosphere is an important parameter controlling the kinetic process of quantum dot evolution, and it was demonstrated that SPA was a viable monitoring technique for quantum dot formation.

I7.25
TEM AND PL STUDIES OF InAs AND $In_{0.9}(Ga/Al)_{0.1}AS$ SELF-ASSEMBLED QUANTUM DOTS ON InP SUBSTRATE. Zhong-zhe Sun, Ju Wu, Feng-qi Liu, Huai-zhe Xu, Yong-hai Chen, Xiao-ling Ye, Wei-hong Jiang, Bo Xu, Zhan-guo Wang, Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, Beijing, PR CHINA.

In this paper, $In_{0.9}Ga_{0.1}As$, $In_{0.9}Al_{0.1}As$ and InAs self-assembled quantum dots (QD) are grown by Stranski-Krastanow growth mode on $In_{0.52}Al_{0.48}As$ lattice-matched to (001)InP substrates by a Riber 32P MBE system. The structural and optical properties were characterized using TEM and PL, respectively. Experimental results reveal obvious effect of ternary composition on QD formation, size distribution and luminescence.
Due to reduction of strain in ternary $In_{0.9}Ga_{0.1}As$, $In_{0.9}Al_{0.1}As$ layer, they show larger critical thickness for quantum dots formation than InAs layer. TEM results show ternary $In_{0.9}(Ga/Al)_{0.1}As$ dots behave relatively larger size (40nm and 80nm) than InAs dots (~34nm). In addition, $In_{0.9}Al_{0.1}As$ dots show larger size, lower density than $In_{0.9}Ga_{0.1}As$ dots. PL results show relatively strong dot luminescence located at around 0.6~0.8 eV, the FWHM of luminescence peaks from $In_{0.9}Ga_{0.1}As$, $In_{0.9}Al_{0.1}As$ and InAs dots are 39, 67 and 142 meV, respectively. We attribute the narrower luminescence linewidth from ternary QDs to low sensitivity of QD ensemble with larger size for size fluctuation. The linewidth from $In_{0.9}Ga_{0.1}As$ is narrower than $In_{0.9}Al_{0.1}As$ due to its higher size homogeneity. Above results show that an appropriate reduction of strain for QD on $In_{0.52}Al_{0.48}As$/InP matrix will be an available path to improve optical property for device applications.

I7.26
PHOTOREFLECTANCE INVESTIGATION OF InAs/GaAs SELF-ASSEMBLED QUANTUM DOTS GROWN BY ALMBE. Mario Geddo, Rolando Ferrini, Giorgio Guizzetti, Maddalena Patrini, INFM-Univ Pavia, Dept of Physics, Pavia, ITALY; Secondo Franchi, Paola Frigeri, CNR-MASPEC Institute, Parma, ITALY.

Although the optical properties of InAs quantum dots (QDs) have been extensively investigated by photoluminescence techniques, very little work has been done on QDs using modulation spectroscopy. In this communication we present a photoreflectance (PR) investigation from 90 K to room temperature of the optical transitions in quantum dots arrays grown by Atomic Layer Molecular Beam Epitaxy (ALMBE). The samples consist of N planes (N=1 to 9) of InAs self-assembled quantum dots (SADs); for N=1 the QDs are capped with a GaAs layer to provide the confinement of carriers, while for N>1 the topmost QDs are uncapped and the QD planes are spaced by 10nm thick GaAs layers.[1] Photoreflectance measurements have been performed in the 0.8-1.5 eV energy range. The optical spectra were analyzed by using typical PR lineshape model characterizing electromodulated signals in bound states such as those in quantum dots and quantum wells.[2] Spectral features connected with optical transitions originating in the QD region of the heterostructures appeared in all spectra, including that of the sample with N=1. Room temperature SAD PR features were located at ~ 1eV with a transition broadening of ~ 30-50 meV and exhibited a temperature behavior similar to the InAs strained band gap. When N was increased from 1 to 2, spectra displayed a significant blue-shift (~ 30 meV) of the SAD PR features; on the other hand a weak red-shift (~ 5 meV) with 30% reduction of the transition broadening appeared when successive layers (up to 9) were added. The evolution of the ground state transition energy vs. the number of stacked layers is discussed considering the combined effects of vertical coupling and Coulomb interaction and evidence is given to the possibility to get an optical characterization of QD heterostructures, even at room temperature, taking advantage of the derivative-like nature of PR technique. [1] P. Frigeri et al. J. Crystal Growth -in press- [2] L. Aigouy et al. Appl. Phys. Lett. 70, 3329 (1997)

I7.27
NANO-PHOTOLUMINESCENCE STUDIES OF SELF-ASSEMBLED QUANTUM DOTS. H. Htoon[1], Hongbin Yu[1], D. Kulik[1], J. Keto[1] and C.K. Shih[1], O. Baklenov[2] and A.L. Holmes Jr.[2]; [1]Department of Physics University of Texas at Austin, Austin TX; [2]Department of Electrical and Computer Engineering, University of Texas at Austin, Austin TX.

Semiconductor quantum dots (QDs), the mesoscopic equivalent of natural atoms, have attracted intense research efforts not only for their similarity to natural atoms in their opto-electronic properties but also for their much richer and more complex characteristics that have no counter parts in atomic physics. In spectroscopic studies of QDs, the most challenging task is to limit the number of QDs in the probing volume and isolate emission lines of a QD from that of an ensemble. By using nano-aperture method and cross-sectional nano PL technique the number of QDs in the probing region can be limited to a hundred or less. Out of the resulting atomic like sharp spectral features from these QDs, the emission lines of a single QD can be further isolated by using the spectroscopic imaging shceme[1]. These techniques allows us to study following physical phenomena of individual QDs: (a) thermally activated inter-dot carrier transfer among neighboring QDs [1] (b) formation and disintegration of multi-particle states manifested by the inter-dot population shuffling[1], and (c) quantum confined stark effect. 1. H. Htoon et al 'Viewing Quantum Dots at Nanometer Scale: Inter-Dot Carrier Shuffling and Multi-Particle States' Submitted to Phys. Rev B.

I7.28
ELECTRICAL PROPERTY OF NANO-SCALE $TiSi_2$ ISLANDS ON Si. Jaehwan Oh, Hoon Ham, Peter Laloli and R.J. Nemanich, Department of Physics, North Carolina State University, Raleigh NC.

Nano-scale $TiSi_2$ islands are formed by electron beam deposition of a few monolayers of titanium film followed by in situ annealing at high temperatures (800-1000°C). The typical island sizes were less than 10 nm. Electrical characteristics of these islands were probed using UHV-STM and ambient conducting tip AFM. The AFM measurements show a different conductivity between islands and substrate as the bias is changed. UHV-STM was used for I-V spectroscopy on these islands and show quantum size effects such as Coulomb Blockade and Coulomb Staircase at room temperature. At higher bias, the I-V spectra also show negative differential resistance (NDR). These effect can be explained in terms of the leakage current between the island and substrate and the tunnel junction.

I7.29
FABRICATION OF EPITAXIAL PYRAMIDAL ISLANDS ON Ge(100) USING Sn/C LITHOGRAPHIC MASKS. Jie Zhang, Douglas J. Swenson, Stephen A. Hackney, Department of Metallurgical and Materials Engineering, Michigan Technological University, Houghton, MI.

A method is described for the molecular beam epitaxial growth of faceted, pyramidal islands on Ge (100) single crystals. The technique involves the initial deposition of spatially modulated, self-assembled Sn islands, which are subsequently surrounded by a continuous C layer during C deposition. The pyramidal Ge islands then form when additional Ge is deposited on top of this Sn/C structure. The Ge islands are epitaxial with the substrate and are bounded by {111} facets. They exhibit height-to-width ratios of about 1:2 to 1:3, and islands with basal widths as small as 200 nm are observed. Compared with the hut/dome morphologies typically observed during coherent strained layer growth of Ge, these pyramidal structures, with their unusually large bases and atypical faceting, appear anomalous and suggest that a unique islanding mechanism may be operative in the present case. By changing the growth conditions of the initial Sn and C layers, it is found that initial deposition of both Sn and C is required in order for pyramidal Ge island formation to occur. Moreover, the Ge island size is observed to scale with the size of the Sn islands in the initial Sn/C structure. These phenomena, as well as the scale and faceting of the Ge islands, are consistent with the hypothesis that during Ge growth, the Sn/C layer acts as a lithographic mask, allowing Ge deposition directly on the substrate through the Sn islands, but precluding the growth of a Ge layer on the C film. Additional evidence for this unique islanding mechanism is discussed, along with a more detailed description of the changes in film morphology with variation in growth conditions.

I7.30
STRAIN RELAXATION AND 3-D CLUSTERING OF HETEROEPITAXIAL SiGe FILMS VIA STRESS-DRIVEN SURFACE EVOLUTION. Cengiz S. Ozkan, Applied Micro Circuits Corporation, Process Development Division, San Diego, CA.

We have studied the strain relaxation and 3-D islanding of heteroepitaxial SiGe thin films grown on Si(001) substrates using low pressure chemical vapor deposition. The flat and defect free as-grown films were subjected to various annealing conditions to induce morphological evolution and eventually 3-D islanding. These films were characterized using AFM and TEM for surface morphology and defects.

I7.31
MORPHOLOGY EVOLUTION IN SILICON-GERMANIUM THIN FILMS-EFFECTS OF THE SIGN OF THE MISFIT STRAIN. B.G. Demczyk, U.S. Air Force Research Laboratory, SNHX, Hanscom AFB, MA; A.H. King and R.J. Gambino, Department of Materials Science and Engineering, State University of New York, Stony Brook, NY.

A study of the surface morphology and interface structure of silicon-germanium films, grown by ultrahigh vacuum chemical vapor deposition on single crystal silicon and germanium substrates was undertaken. Two independent, but competing factors combine to determine the resulting film morphology developed in these films. The minimization of surface energy was seen to control the initial film coverage of the substrate by the deposit. Absent any film-substrate misfit strain, systems tend to maximize (111) surface area at the expense of other orientations, such as (001). When misfit strain is present, the systems seek to relieve it through the formation of misfit dislocations. Although it is to be expected that misfit dislocation formation is facilitated by large strains, it was found that the sign of the strain is equally important. Systems strained to an equal extent, but oppositely directed, develop vastly different surface morphologies. In particular, compressively strained films are prone to the formation of surface undulations, while films in tension are not. The latter films are, however, much more heavily defected. These results are discussed in light of the mechanistics of dislocation formation in semiconductor structures.

I7.32
IN-SITU TEM OF MBE GE GROWTH ON SILICON. William L. Henstrom, Chaun-Pu Liu, Peter D. Miller, University of Illinois at Urbana/Champaign, Dept. of Physics, Urbana, IL; J. Murray Gibson, Argonne National Lab, Material Science Divsion, Argonne, IL.

The investigation into the growth of strain induced, self-assembled, quantum dots has been an area of high interest in the last few years. Using *in-situ* UHV TEM, we have studied the evolution of MBE deposited Ge domes on Si (100) during thermal annealing at different temperatures and under varing conditions. A powerful tool is the TEM dark-field strain contrast measurement of the strain in individual domes. When we compare our measurements with samples made by CVD, we find differences in both size and strain distributions for the Ge domes.

I7.33
Abstract Withdrawn.

I7.34
PULSED MAGNETIC FIELD INDUCED 3-D ISLANDING OF OXYGEN CONTAINED CLUSTERS IN Cz-Si CRYSTALS. Mark N. Levin, Voronezh State Univ, Nuclear Phys. Dept, Voronezh, RUSSIA; Boris A. Zon, Voronezh State Univ, Dept of Math. Phys., Voronezh, RUSSIA.

The effect of magnetic field induced generation of oxygen-vacancy (O-V) centers (A-like centers) in silicon crystals grown by Czochralski method (Cz-Si) was reported earlier [1]. Now we present the picture of secondary defect formation in Cz-Si crystals after the pulsed magnetic field (PMF) treatment. It was found out that short-term effects of PMF initiate long-term low-temperature decay of a supersaturated solid solution of oxygen in Cz-Si crystals. It results in generation of oxygen-containing defects in the form of O-V centers and more complicated $Si_xO_yV_z$ complexes. The PMF-induced microstructure evolution culminates in the formation of spatially ordered oxygen-vacancy clusters and/or the oxide precipitates, depending on the origin defects present in the crystal. STM and SEM studies of the surface topology of the Cz-Si crystals with layer-by-layer etching showed that PMF-induced effects appear very different in the near-surface layers and in the depth of the crystal. It results in precipitation of oxide phases in the near- surface layers of the crystal, where the process facilitates by the original structural defects that can serve as primary nucleation centers. In the bulk of the Cz-Si crystals with higher structural perfection the action of PMF results in self-organized formation of regular 3-D structures of nanometer scale. All the processes take place at room temperature. The Cz-Si crystals with the regular 3-D structure of $Si_xO_yV_z$ clusters emit light in the green region of spectrum under the UV laser excitation. 1. M.N. Levin, B.A. Zon, MRS Spring Meet. Abstr., G2.9, 1999

I7.35
HIGH RESOLUTION ANALYTICAL TEM INVESTIGATION OF THE MICROSTRUCTURE AND COMPOSITIONS OF INAS QUANTUM DOTS ON GaAs. M.A. Al-Khafaji, A.G. Cullis, M. Hopkinson, C.R. Whitehouse, Department of Electrical and Electronic Engineering, University of Sheffield, Sheffield, UNITED KINGDOM; M.S. Skolnick, Department of Physics and Astronomy, University of Sheffield, Sheffield, UNITED KINGDOM.

In this study, various Analytical Field Emission Transmission Electron Microscopy techniques were used to investigate the chemical composition and microstructure of different configurations of InAs self-assembled quantum dots on (001) GaAs. Selected samples were grown by molecular beam epitaxy under a range of conditions to give a variety of sizes and separations of the quantum dots: both capped and uncapped samples were prepared. Nanoscale composition variations within the dots and across wetting layers were measured using electron energy loss elemental mapping in both imaging and spectroscopy modes. Measurements using energy loss imaging were carefully performed to eliminate the potential deleterious effects of overlapping strain contrast. Energy dispersive X-ray spectroscopy with $<$1nm electron probes was also employed to produce composition profiles on the same scale. The results were correlated with the dimensions of the dots determined by high resolution imaging and complementary atomic force microscopy using high aspect-ratio tips. The presentation will correlate composition profiles across the different structures with changes in growth conditions. The variation of quantum dot density and morphology with growth rate will also be discussed.

SESSION I8/N9: JOINT SESSION: REAL-TIME IN-SITU STUDIES ON 3-D ISLANDING

Chair: Stephen J. Pennycook
Thursday Morning, December 2, 1999
Wellesley (M)

8:30 AM *I8.1/N9.1
TRANSITION STATES BETWEEN PYRAMIDS AND DOMES DURING ISLAND GROWTH IN THE Ge/Si SYSTEM. F.M. Ross, R.M. Tromp, J. Tersoff and M. Reuter, IBM Research Division, T.J. Watson Research Center, Yorktown Heights, NY.

We have examined the growth and evolution of self-assembled Ge and GeSi islands on Si(001) using UHV transmission electron microscopy

and low energy electron microscopy. The Ge/Si(001) system is of great interest because of the existence of two island shapes, shallow pyramids and more complex domes with steeper facets. In situ electron microscopy allows us to observe the development of these island shapes at video rate during growth by chemical vapour deposition, enabling us to distinguish between models for island formation.
After the nucleation of pyramidal islands, we observe a coarsening process which dramatically reduces the island density and increases the mean island volume. Surviving islands which reach a critical volume then change from the pyramid to the dome shape. We find that this shape change takes place slowly with the island passing through numerous asymmetric transition states having increasing numbers of higher angle facets. These asymmetric transition shapes can persist for several minutes, but they are temperature dependent and transform reversibly to the final dome shape during cooling. We can explain all our in situ results by using an anomalous coarsening model in which a process similar to Ostwald ripening occurs amongst an ensemble of islands whose equilibrium shape (pyramid, dome or transition shape) depends on volume. In this presentation we will show videos of island nucleation and growth and we will discuss this model. We will also describe how island development is modified by the strain fields of neighbouring islands and substrate dislocations. This is of interest since the use of substrate strain fields to pattern islands may allow us to develop uniform arrays of islands for new electronic applications.

9:00 AM *I8.2/N9.2
EPITAXIAL GROWTH OF GERMANIUM ON Si(001) - STUDIES BY HIGH TEMPERATURE STM DURING GROWTH. Bert Voigtlander and Martin Kastner, Institut für Grenzflachenforschung und Vakuumphysik, Forschungszentrum Julich, GERMANY.

We use a scanning tunneling microscope (STM) capable of imaging the growing layer during MBE-growth at high temperatures. This method (MBSTM) opens the possibility to follow MBE growth processes dynamically on the atomic scale and gives access to the evolution of specific features during growth. The method is applied to study the epitaxial growth of Germanium on Si(100). The periodicity of the (2×N) reconstruction of two-dimensional Ge layers on Si(001) is measured as function of the Ge coverage. The strain energy, which increases with increasing coverage, is the driving force for the formation of the strain relieving (2×N) reconstruction trenches and Si/Ge intermixing. A quantitative comparison to total energy calculations predicting the periodicity of the (2×N) reconstruction with the experimental results is used to estimate the amount of Si-Ge intermixing near the surface. The evolution of size and shape of individual {105} faceted Ge islands (hut cluster) on Si(001) is measured during growth. A slower growth rate is observed when an island grows to larger sizes. This behavior can be explained by self-limiting growth. A kinetic growth model involving a nucleation barrier for each repeated growth of a new atomic layer on the {105} facets agrees with the experimental results for the evolution of the island volume. The experimentally observed shape transition from nearly square shaped islands to elongated islands is described by the kinetic growth model. Some of the results will be presented on videotape.

9:30 AM *I8.3/N9.3
CHEMICAL ORDERING AT AND NEAR SURFACES: A UNIQUE INPUT OF GRAZING INCIDENCE X-RAY DIFFRACTION Michele Sauvage-Simkin, LURE, Orsay, FRANCE and Laboratoire de Minèralogie-Cristallographie, Paris, FRANCE.

The growth of alloyed materials by surface techniques has given evidence for the dramatic effect of surface segregation processes on the compositional homogeneity of the epilayers. The resulting composition profiles can be modelized as a function of thermodynamical and kinetic parameters. However, the influence of reconstructions possibly stabilizing a given surface composition has not been introduced into the energy balance although, in the particular case of III-V semiconductor ternary alloys (In,Ga)As strained on GaAs(001), specific commensurate 2x3 or incommensurate 2xn ($2.5<n<3$) were observed. Surface X-ray diffraction measurements performed in-situ on MBE grown (In,Ga)As alloys and on submonolayer In deposits, strained on GaAs(001), have enabled to ascribe the 2x3 reconstruction to a chemically ordered distribution of cations in the different subsurface sites defined by the arsenic arrangement in the very top layers. The surface composition was thus found locked at the value $In-0.67Ga-0.33As$ with a minimal strain in the surface In-As and Ga-As bonds. Incommensurate 2xn surfaces could be produced by forcing the indium surface concentration out of this nominal value and it will be shown that a full account of the diffraction pattern is obtained by considering, in a diffuse scattering formalism, a probabilistic distribution of either indium depleted or indium enriched faults in the 2x3 perfect order. In a proper temperature range, a direct correlation between the surface stoichiometry and the discommensuration can be established. In order to address the influence of the average strain on the segregation trend, the results obtained on the 2x4 reconstructed ternary alloy $In-0.53Ga-0.47As$ adapted on InP(001) will be discussed. Being sensitive to long range order among chemical species at and near the surface, grazing incidence X-ray diffraction is an optimal tool to address the atomic arrangements in the early stages of heteroepitaxial growth and to complement the information derived from local probes such as scanning tunneling microscopy.

10:15 AM *I8.4/N9.4
IN-SITU MEASUREMENTS OF STRESS RELAXATION DURING STRAINED LAYER HETEROEPITAXY. E. Chason, J. Yin, K. Tetz, R. Beresford, E. Chen, D. Paine, L.B. Freund, Brown University, Providence, RI; J.A. Floro, Sandia National Laboratories, Albuquerque, NM.

Stress plays a critical role in determing the evolution and the properties of heteroepitaxial layers. Stress-induced morphological changes such as island formation can prevent the formation of sharp interfaces. Dislocations that form to relieve the stress can severely degrade the electronic properties of the layer. Although there has been much work done on the energetics of stress relaxation, the kinetics of stress relaxation have not been studied as intensively because of the difficulty of obtaining real-time data. In this talk, we will discuss measurements of dislocation-mediated stress relaxation in layers of InGaAs grown on GaAs (001) performed during growth. These results were obtained using a novel wafer-curvature based technique optimized for in situ studies. At high temperature or stress, the layers relax continuously above the critical thickness, while for low temperatures or stress, the films grow pseudomorphically over a much larger region of metastability before relaxing rapidly. In addition, we find that relaxation occurs without additional growth above a certain thickness. By comparing measurements made with and without growth interrupts, the relaxation at constant thickness can be separated from the relaxation during growth. The degree of relaxation induced by growth interrupts at constant temperature and at elevated temperature is compared with the stress evolution during continuous growth. Results are interpreted in terms of models of dislocation-mediated relaxation. Portions of this work were performed at Sandia National Laboratory and supported by the United States Department of Energy under contract DE-AC04-94AL8500.

10:45 AM *I8.5/N9.5
REAL-TIME X-RAY STUDIES OF MORPHOLOGICAL TRANSITIONS DURING MOCVD GROWTH OF GaN. G.B. Stephenson[a], M.V. Ramana Murty[a], J.A. Eastman[a], C. Thompson[a,b], A. Munkholm[c], P. Fini[d], O. Auciello[a], R. Jothilingam[d], S.P. DenBaars[d] and J.S. Speck[d]; [a]Materials Science Div., Argonne National Laboratory, Argonne, IL; [b]Dept. of Physics, Northern Illinois University, Dekalb, IL; [c]Chemistry Div., Argonne National Laboratory, Argonne, IL; [d]Materials Dept., University of California, Santa Barbara, CA.

The competition between deposition rate, surface diffusion, adatom attachment at steps, and nucleation of islands can lead to a variety of surface morphological transitions during crystal growth. We have used real-time grazing-incidence x-ray scattering to observe the growth modes of GaN(0001) and the faceting of vicinal surfaces during metal-organic chemical vapor deposition (MOCVD). We have observed transitions between the classical homoepitaxial growth modes (step-flow, layer-by-layer, and three-dimensional) as a function of growth rate and temperature on singular GaN(0001) surfaces [1]. On vicinal surfaces, high-temperature growth leads to faceting (step bunching), while subsequent annealing without growth produces an ordered staircase of monolayer-height steps. This behavior will be contrasted with that of GaAs(001), for which growth favors step ordering.
[1] G.B. Stephenson *et al.*, *Appl. Phys. Lett.* **74**, 3326 (1999).
This work was supported by the U.S. DOE, BES–DMS under contract W-31-109-ENG-38, the NSF under grant DMR–9704201, and the State of Illinois under HECA.

11:15 AM *I8.6/N9.6

DAVID TURNBULL AWARD LECTURE

ATOMIC-LEVEL CONTROL DURING FILM GROWTH UNDER HIGHLY KINETICALLY CONSTRAINED CONDITIONS: H-MEDIATION AND ULTRA-HIGH DOPING IN $Si_{1-x}Ge_x$ GAS-SOURCE MBE. J.E. Greene, Univ of Illinois-Urbana, Materials Science Dept and MRL, Urbana, IL.

Surface reaction pathways and kinetics of $Si_{1-x}Ge_x$ growth on Si(001) by both gas-source MBE (GS-MBE) and atomic-layer epitaxy (ALE) from Si_2H_6/Ge_2H_6 mixtures have been investigated using a combination of $in-situ$ RHEED, EELS, STM, STS, TPD, and AES

together with post-deposition TEM, HR-XRD, XTEM, and electronic transport measurements. Film growth data are well described by models containing separate reaction steps for dissociative chemisorption, surface reactions, and hydrogen desorption. For UV-photostimulated ALE, hydrogen termination provides internally self-limiting kinetics and allows epitaxial growth at room temperature and below.

The results of isotopically-tagged D_2 temperature-programmed desorption (TPD) experiments were used to model temperature-dependent H-mediated effects of high B coverages on the growth kinetics of B ultra-high doped $Si_{1-x}Ge_x(001)$, up to $1.5x10^{22}$ cm^{-3} (30 at%), through changes in B-induced surface reconstruction and back-bond charge transfer, and to determine Ge segregation kinetics as a function of x and steady-state H coverage during GS-MBE. Excess incorporated B does not precipitate out of solution as commonly supposed. Rather, our recent NEXAFS and HR-XRD results, carried out at the Synchrotron Radiation Center in Stoughton, show it is incorporated as sp^2 bonded dimers with trigonal symmetry on substitutional Si sites. The dimers are bond-saturated and thus electrically neutral. Further, they have very low charge scattering cross-sections.