SYMPOSIUM I

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

November 29 – December 2, 1999

Chairs

David M. Follstaedt
Nanostructure & Semiconductor Physics Dept
Sandia National Labs
MS 1056
Albuquerque, NM 87185
505-844-2102

Bruce A. Joyce
Dept of Physics
Imperial College
The Blackett Laboratory
London, SW7 2BZ
UNITED KINGDOM
44-171-5946694

Angelo Mascarenhas
Center for Basic Sciences
National Renewable Energy Lab
Golden, CO 80401
303-384-6608

Tohru Suzuki
NEC Corporation
Opto-Electronics &
High-Frequency Device
Tsukuba, 305 JAPAN
81-298-50-1525

Symposium Support
Army Research Office
National Renewable Energy Laboratory

Proceedings published as Volume 583
of the Materials Research Society
Symposium Proceedings Series.

*Invited paper
SESSION II: QUANTUM DOTS I
Chair: Ivo De Vreese and Ray D. Trestian
Monday Morning, November 29, 1999
Wellesley [M]

8:30 AM II.1
MOLECULAR BEAM EPITAXY STUDY OF 3D ISLANDING IN THE InGaAs/GaAs SYSTEM. P. Bieke, J.B. Smidtters, H. Yang, C.L. Workman and J.G. Salomo, Physics Dept, University of Arkansas, Fayetteville, AR.

We present the results of an investigation of the 3D islanding in the highly mismatched InAs/GaAs 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 described as Stranski-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 [AlGa]As barriers can be designed to achieve large tunability of the quantum dots emission energy.

8:45 AM II.2
THE SHAPE OF InAs SELF-ASSEMBLED QUANTUM DOTS GROWN ON InGaAs/InP. Sukhee Youn, Youngho Moon, Tae-Won Lee, and Byoung 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 themselves 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 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 InGaAs/GaAs 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 (~100 nm wide and ~10 nm high) due to the smaller misfit strain compared to InAs/GaAs dots, enabled us to identify the [116] facets by atomic force microscopy. Moreover, the [116]-faceted InAs dots were elongated along either [110] or [110] to form parallelogram-based dots, analogous to but clusters observed in SiGe/Si quantum dots, however, due to their unique geometry with [116] facets they looked as if they were all elongated along [110] direction. We believe that these particular faceted quantum dots have a hypothetical rhombohedral based dots. Some parallelogram-based dots were found to have a smaller 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 [116]-faceted dots will be presented.

9:00 AM II.3
HIGH RESOLUTION ANALYSIS OF EMBEDDED QUANTUM DOTS. Alan Harvey, U of MEST, Dept of Physics, Helen Drinkwater 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 the 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 specimen section. The results are compared with STEM analyses of InAs dots in a GaAs matrix.

9:15 AM II.4
Abstract Withdrawn.

9:30 AM II.5
GROWTH PHENOMENA OF QUANTUM DOT STRUCTURES IN THE InGaAs SYSTEM INVESTIGATED BY TEM TECHNIQUES. Peter Werner, MRS-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 years, the generation of QDs has been attempted using different techniques. However, there was a breakthrough initiated by employing self-organizing mechanisms during the epitaxial growth of lattice-mismatched semiconductor alloys forming 2- and 3-dimensional arrays of quantum dots based on the Stranisky-Krastanov 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 focused on the formation and properties of InGaAs islands (dots) in a GaAs matrix, via a system showing properties similar to those of other material 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 emit light in the range of 1.1 mm, the development is directed to structures emitting light at 1.3 mm and 1.5 mm at RT. The talk will point out some structural/growth possibilities to reach this goal.

The 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 II.6

Tuns as well as micro-photoconductivity studies of InP/GaNP quantum dots (QDs) fabricated via the Stransky-Krastanov 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 through a transparent Schottky barrier on the surface of the GaNP 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 Fermi level is shifted to lower energies and individual lines in the multiplet sequentially disappear, until 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 eV broad lines split up into several very sharp lines, with FWHM values comparable to the resolution of our spectrometer system (5 k100 eV).

In the extreme limit of peak appearance we detect what we believe is an isolated electron-hole pair. In the other limit of bias conditions we estimate that 1.5-20 electrons occupy the QD, leading to the multiplet of lines over the spectral range of 4646 eV. 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 consistent picture is finally obtained when one applies the electron recombination per added electron, which from capacitance spectroscopy has been estimated to be around 10 meV per electron [3]. These observations present an intriguing cyclic system which allows controlled tuning of the occupancy of a single QD in the range 0-19 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 be used as donors but may also allow studies that go beyond the optical properties that we have a hook by which we may tune the occupancy of a single, artificial, atom. References [1] Hesseman et al, APL 69, 7441 (1996) [2] Pryor et al, RPH5, 10048 (1997) [3] Anzold et al, APL 67, 3016 (1995)

11:00 AM II.7
THE EFFECT OF INTERMITTENCY ON SELF-ASSEMBLED QUANTUM DOT FORMATION. Hyungwoon Jeong, Albert-Ludwig-Universität, University of Notre Dame, Department of
Physics, Notre Dame, IN.

Interspreading is known to affect both 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 be related to a new formation of SAQD, are absent. We discuss how the degree of alloying affect the phase diagram of SAQD formation. Finally, the results are compared with high temperature growth experiments, exhibiting interspreading and alloying during the formation of strained islands.

11:15 AM IL 8
CHARACTERIZATION OF InAs QUANTUM BOXES USING CROSS-SECTIONAL SCANNING TUNNELING MICROSCOPY.

Cross-sectional 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 boundary versus the volume of dots and the distance between two successive arrays of InAs dots is modeled using a 3D 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 IL 9
InAs QUANTUM DOTS ON SILICON. L. Hansen, F. Bessing, A. Ankudinov, A. Wang.

Embedding of photonic 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. We have performed a systematic study on the specific 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, whereas 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 minimum of 10^11 cm^-2 of dots 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 InQDs on Si, protected by an additional ZnO cap against surface oxidation, where we observe an PL peak at 1.2-1.3 μm, a wavelength range which is very interesting for optical fiber applications.


SESSION 12: SPONTANEOUS ORDERING IN SEMICONDUCTOR ALLOYS.

Chairs: Sayen K. Deb and Rebecca L. Forrest
Monday Afternoon, November 29, 1999

Wellstone [M]

1:30 PM *D12
X-RAY AND TEM STUDIES OF ORDERING IN TERNARY SEMICONDUCTOR ALLOYS. Joseph Kulik, Univ of Houston, Texas Center for Superconductivity (TCSCH) and Dept of Physics, Houston, TX; Rebecca Forrest, Univ of Houston, Dept of Physics, Houston, TX and UCLA, Los Angeles, CA; Jinhuan Li, Texas A&M, College Station, TX; David 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 supersaturated formation) and faulting - both twin and stacking disorder - in ternary semiconductor alloys of the generic form III$_1$V$_2$ (V = In, Ga) and III$_1$V$_2$ (V = Al, Ga) [1,2]. We have also undertaken experiments on the tetragonally strained alloys GaInP and Al$_x$Ga$_{1-x}$As to recover the degree of order and to demonstrate the presence of both short-range and long-range ordering. We have also initiated asymptotic X-ray studies of orientational ordering in GaInP supplied by NREL (Z. Zhang, A. Maschkehrs). In all of these studies we are concerned with the quantitative evaluation of the degree of order, and its relationship to electronic properties, 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 D12
FIRST OBSERVATION OF ATOMIC LONG-RANGE ORDERING IN METAL-OXIDE BASED ZnMgO WIDE BAND GAP HETEROSTRUCUTURES. R.D. Vajape, S. Choopun, D.M. Chalk, S.B. Ogale, R.P. Sharma and T. Venkatesan, CSR, Dept of Physics, University of Maryland, College Park, MD; A. Hixson, 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 future 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 (3.08 eV) ZnMgO alloy semiconductor thin films grown on sapphire (0001) by pulsed laser deposition. In 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 for the wurtzite structure. Under optimum growth conditions, Zn and Mg preferentially occupy high substrate. 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 Murray (DMR 982521) and NSF contract supervised by Dr. Khodas.

2:15 PM D13

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 CuIn-Se$_2$ material system have indicated that ordering of the cation sublattice along the [001] direction in CuInAs$_2$ structure is necessarily incoherent 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, but never before in the CuInSe$_2$ system. Current evidence for the layered-tetragonal structure is provided by two methods. X-ray diffraction and specular reflection exhibits an unusually prominent series of diffraction peaks at 20 angles of 15.45°, 47°, 64.1° and 80.9°, in addition to the A$_1$ mode at 175 cm$^{-1}$ and the B$_1$ (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 structure metrology on 3D island formation will be described in detail, emphasizing the observation that their ordering into self-assembled arrays occurs only in the case of copper excess. S.-H. Wei, et al., Physical Review B 45(5), 2332-2336 (1992). S. Xu, et al., 11th International Conference on Terahertz and Midinfrared Compounds, 929-932, Salford, England, (1997).
CoPt 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 disorder is caused by an increase in the GaIn ratio 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 the Te is postulated to be responsible for the disordering. Perhaps the most exciting development in this area is the use of the in-situ electron group V elements Sb to control the surface reconstruction and, hence, the order parameter and the GaInP bandgap energy. Modulation of the TE growth flow rate has shown growth can be induced to produce a heterostructure with a 135 meV bandgap difference between two layers having the same composition, one grown with and the other without any Te.

**3:30 PM 12.5**
**SPATIALLY-RESOLVED PHOTOEMISSION IN SPONTANEOUSLY-ORDERED GaInP.** J. Smith, H. M. Cheong, B.D. Hiegel, J.P. Geisz, J.M. Olson, L.L. Knezewski and A. Macashevska, NREL, Golden, CO.

The low-temperature (5K) photoluminescence (PL) of partly-ordered GaInP is spatially resolved using high-resolution (~0.7nm) scanning optical microscopy combined with high-resolution scanning electron microscopy (~40μm), revealing the spatial variation in band gap energy and the spatial origin of the ordering. The ordering of the ordering is induced by photoemission and the microscopically ordered (quantum-dot-like) narrow splices which appear when varying the growth or optical properties, often below the critical point of a single ordered domain. The large number of samples taken within a microscopically ordered area allow a detailed look at the statistical variations in bandgap energy and line shape. A systematic study of a series of samples where the optical parameters varies from Δn ≈ 0.05 to 0.4 shows that for highly ordered samples, the statistical distribution of the excitonic energy and linewidth shows 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 12.6**
**CORRELATION OF InGaP(III) SURFACE STRUCTURE DURING GROWTH AND CuPt-B-TYPE BULK ORDERING.** M. Zem, J-T. Zettler, W. Rüdiger, NIKF, München, Germany, A. Skreibert, Department of Physics, University of Toronto, Toronto, Canada, P. Korpas, M. Weyers, FB 5-Inst. f. Hochfrequenztechnik, Berlin, Germany, B. L. Summer and T. Lorents, Depart of Solid State Physics, Lund University, Lund, Sweden.

The mechanism causing CuPt-B-type ordering in InGaP grown lattice-matched to GaAs is studied by in-situ 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 determined by different surface reconstructions. In the experiments, the bulk contribution to the reflectance anisotropy, caused by the loss of symmetry due to the InGaP bulk ordering, was determined. Therefore, the superimposed surface contribution to the RHEED spectra could be extracted, which was identified for all growth conditions (varying temperature, growth rate, doping level, and sample orientation) as a superposition of only two characteristic types of spots, corresponding to a [21c] and [24d] surface reconstruction, respectively. Bulk ordering only occurs when InGaP growth is performed under phosphorus-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 [21c] and [24d] in [21c] mirror symmetry at the growth surface trigger the bulk ordering driven by an energy gain of 26 eV/surface monolayer to the TE calculations.

**4:15 PM 12.7**
**DOMAIN SHAPING ANALYSIS of CuPt-B ORDERED GaAlAs/GaAs HETEROSTRUCTURE PHASES BY ELECTRON MICROSCOPY.** C.D. Moore, R.R. Hess, C.L. Forest, and M.S. Goscinsky, 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 GaAlAs/GaAs 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 combination with transmission electron microscopy, allows more detailed crystallographic information about the structure of larger domains to be obtained. Maps of the growth order in the ordered domains from ~1 μm GaAlAs 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 0.08. The shape of the θ [1 0 1] crystal truncation rod has a circular cross section; this is in agreement with observations from transmission electron diffraction patterns taken along the same crystalllographic direction. 10 μm GaAlAs grown on GaAs tilted 6 degrees toward the [1 0 0] grow reciprocal space maps that represent domains elongated and tilted by a few degrees from the [1 0 0] growth direction. Three-dimensional mapping indicates that the ordered domains are more elongated along the [1 0 1] than the [1 0 0] direction. Domain morphology will be discussed in terms of growth kinetics and substrate miscut.

**4:30 PM 12.8**
**CuPt ORDERING SIGNATURES OF PHONONS in GaInP.** Francesco Alasia, Univ Autonoma de Barcelona, Dept of Physics, Bellaterra, SPAIN; Hycnisk M. Cheong, National Renewable Energy Laboratory, Golden, CO; Narciso Mestres, ICMM-CSIC, Bellaterra, SPAIN; Angelo Macashevska, National Renewable Energy Laboratory, Golden, CO; Jordi Pratпал, Univ Autonoma de Barcelona, Dept of Physics, Bellaterra, SPAIN.

During the following ten years after spontaneous ordering was first observed in the GaInP alloys most of the studies on optical properties were focused on analyzing the evidence of ordering on the electronic states. The changes induced by ordering in lattice dynamics were found to be 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 samples has permitted us to gain a remarkable amount of experimental evidence for ordering effects on the photon spectra. In this communication we present a comprehensive overview of spectroscopic measurements of phonons in ordered GaInP. The major signature of CuPt ordering in the Raman spectra is the emergence of new peaks in both the acoustic and the optical region. 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 13: QUANTUM DOTS & WAVES**

**8:00 AM E3.1**
**SELF-ASSEMBLED InAlAs/GaAs QUANTUM DOTS GROWN BY MOVCD.** Jae-Hyun Ryu, Utku Chowdhary and Russell D. Dupuis, The University of Texas at Austin, Microelectronics Research Center, Austin, TX; Cheava V. Reddy and Venkatesh Naragamurti, Harvard University, Division of Engineering and Applied Sciences, Cambridge, MA; David T. Mochs and Robert Hall, The University of Virginia, Department of Materials Science and Engineering, Charlottesville, VA.

We have grown self-assembled InAlAs/GaAs quantum dots (QDs) embedded in GaP cladding layers using low-pressure metalorganic chemical vapor deposition (LP-MOVCD). InAlAs/GaP QDs were grown in the Struycken fast-flow (SFF) mode using a 100 mm 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 flux ratios of III elements, V/III ratios, growth temperatures (200-700°C), and growth sequence. The QDs were grown in an E-Beam CSI 200 reactive tool using trimethylgallium, trimethylaluminum, and trimethylammonium as group-III precursors and PH3 for the group-V precursor. The flux rate for the group III precursors were reduced in order to achieve monolayer coverage of the growth rate for the growth of InAlAs/GaP 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. The optimized growth conditions, 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 of 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 E1.2 ENERGY ANALYSIS FOR HETEROEPITAXIAL FILM-
SUBSTRATE SYSTEMS WITH AN ARRAY OF SELF-
ASSEMBLED QUANTUM DOTS. Chenghui Chiu, Institute of
Materials Research and Engineering, SINGAPORE.

The nanostructure 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, for investigating the free energy of a heteroepitaxial system with an array of QDs on the surface. The method provides an efficient way for determining how the free energy varies with the structure of the quantum 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 acting on the heteroepitaxial system. The forces include the mismatch strains between the film and 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 hetero-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 E1.3 INTERDIFFUSION AND SEGREGATION IN STACKED
InAs/GaAs QUANTUM DOTS. B. Liu, R.S. Goldman, Dept. of
Materials Science and Engineering, University of Michigan, Ann
Arbor, M., E. J. Bakr, 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 of wetting layer, island nucleation results in the formation of self-assembled quantum dots. Stacking of 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 (STM) and scanning tunneling spectroscopy (STS), 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 observed interdiffusion layers of In/Ga with 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 for segregation processes are apparent. Such interdiffusion processes in the wetting layer may also affect the lateral extension between columns of dot stacks, thereby providing a means of producing ideal 3D arrays of stacked quantum dots.

9:15 AM E1.4 THE STRUCTURE OF CAPPED AND UNCAPPED InAs/GaAs
QUANTUM DOTS. Dun Zou, D. W. Parker, *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 shape, size, 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 QDs is controlled not only by the QD but also by strain. The capping process also change the QD 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 morphology down to the atomic scale. The ultrafine nature of unalloyed 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 E1.5 STRESS, SURFACE KINETIC PROCESSES, METASTABILITY,
AND SELF-ORDERING IN SEMICONDUCTOR EPITAXY.
Anupam Mishra, 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 determining the formation of metamorphic 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 E1.6 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 Bakkenov, 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 (STM) studies of InGaAs self-assembled quantum dots (QDs) grown using migration enhanced epitaxy (MEE). Samples were cleaved in situ to reveal a section of one of the two circular InGaAs quantum well regions on the QDs. For the 10 ML QDs, we exhibit truncated-triangular shapes with well-defined facets on both (110) and (111) 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 (111) 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 (111) projection. Most importantly, the composition of the InGaAs quantum dots is 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 homogeneous consistent with an inverted-triangle shape of In-rich core in the QD.

10:45 AM E1.7 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 

167
thermodynamics and kinetics of island growth. The shape of the composition profile within the quantum dot may be understood from simple and rather 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 D.8
VERTICAL AND LATERAL CORRELATIONS IN SELF-ORGANISED QUANTUM DOT SUPERLATTICES.
G. Springholz, M. Pinczóls, V. Holy, G. Bauer, Institut füer 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. This makes already built-up lateral 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 fac-like ABCABC vertical dot stacking sequence and nearly perfect hexagonal lateral ordering [2] in the PbSe/PbTe/InSb (111) superlattice system.


11:15 AM E.9
InAs QUANTUM DOTS IN A Si MATRIX: GROWTH AND PROPERTIES.
George E. Cirlin, Nikolai K. Polyakov, Vassili N. Petrov, Institute for Analytical Instrumentation, St. Petersburg, RUSSIA; Dmitri V. Denisov, Boris V. Volkov, Victor M. Usinov, Zhores I. Alferov Physics-Technical Institute, Peterburg, Russia, Nikolai N. Ledentsov, Robert Heitz, Dieter Bimberg, Technical University, Berlin, GERMANY; Nikolai D. Zakharov, Peter Werner, Max-Planck Institute for Microstructure Physics, Halle, GERMANY.

Self-organization 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 - IV (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 lead to significant progress as these nanostructures provide indirect band alignment both in k and in real space. In order to increase the 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 offer a possibility to overcome the problems of strong lattice mismatch and formation of antiphase domains inherent for the growth of thick III-V epitaxial QDs on Si wafer. We have used as a model growth conditions InAs/Si heteroepitaxial growth proceeds via Vickers' layer-by-layer 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 (uncovered islands). We have found that the critical lateral size of the coherent Si-nucleation-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 SiGe that will form SiGe/Si heteroepitaxy results in the complete removal of the dislocated islands with the formation of p+ islands, whereas 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 1.3-1.6 eV region. The pronounced excitation dependence of the PL peak position and a decay time of order of 100-400 ns were observed. The electronic structure of InAs/Si QDs is discussed in view of available band offset information.

11:30 AM F.10
MBE GROWTH: STRUCTURAL AND OPTICAL CHARACTERIZATION OF InAs/InGaAs SELF-ORGANIZED QUANTUM DOTS. Victor M. Usinov, Alexey E. Zhukov, Alexey R. Kovysh, Nikolai A. Mykev, Sergei S. Mikhin, Yuri G. Musikhin, Andrey F. Tantsul'nikov, Boris V. Volkov, Denis A. Bedzheva, Mikhail V. Maximov, St. Petersburg State University, Russia; and Victor M. Usinov, Yaroslav I. Alferov Physics-Technical Institute, St. Petersburg, RUSSIA; Nikolai N. Ledentsov, Dieter Bimberg, Technical University of Berlin, Berlin, GERMANY.

InAs quantum dots 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 microns emission from InAs QDs is to overgrow them with a n-type AlGaAs layer. In the present work we study structural and optical properties of InAs/InGaAs QD structures grown by MBE on GaAs substrates using transmission electron microscopy (TEM), photoluminescence (PL) and electroluminescence (EL). We show that the reason for the increase in the PL wavelength is the phase separation of the InGaAs alloy stimulated by the InAs islands and the effective mass transition by changing a minor role. As the result of the local composition modulation, the effective volume of the 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 n-type layer we notice 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 I: COMPOSITION MODULATION IN SEMICONDUCTOR ALLOYS
Chair: Simon C. Moss and Gerald B. Stringfellow Tuesday Afternoon, November 30, 1999 Wellesley (M)

1:30 PM F.1
KINETIC INSTABILITY OF SEMICONDUCTOR ALLOY GROWTH. Iba P. Ignatova, Vladimir G. Myasnikov, Vitali A. Shchukin, Il’iche Institute, St. Petersburg, RUSSIA; Alexei A. Mironov, Richard F. Walsie, University of California, Department of Physics and Astronomy, Irvine, CA.

Semiconductor alloy epilayers 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 course of growth. We suggest a concept of semiconductor alloy decomposition due to the kinetically induced 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-plan wave vectors of the most unstable mode of composition fluctuations which differ from elastically soft directions [100] and [001]. It opens a possibility for formation of self-organized superlattices oriented in different directions.

2:00 PM F.2

Self-organized lateral composition modulations, which spontaneously form during the epitaxial growth of short-period strained-layer superlattices (SPLS), 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 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 SPLS grown by molecular beam epitaxy on InP substrates. The results have indicated that changing the sign of the optical system between the SPLS and substrates changes the character of the modulations. SPLS grown under moderate global tension exhibit modulations simultaneously along two directions close to c 310>,
inclined \( \approx 2^\circ \) either side of \([110]\). SPS growth under moderate compression exhibit modulations simultaneously along directions close to both the c-axis \( < 110 > \) and \( < 110 > \) 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 indicate 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 highlights the need to further investigate the role of surface segregation on single modulation direction can be selected, enabling greater control of the modulation process for the formation of quantum wire arrays.

2:30 PM 14.3


Lateral composition and morphological modulations can form during the heteroepitaxial growth of misfitting multilayer films, as recently observed in InAs/AIAs, InGaP/InGaAsP, InAs/GaAs, InGaP/GaAs, and SiGe multilayers. We examine the growth 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 interfacial part of the total free energy, which promote the transition 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 the morpohological 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 14.4

Stability of Perturbed Growth Fronts to Stress-Induced Mobility Variations. Jennifer F. Sage, Harvard University, Department of Physics, Cambridge, MA; William Burvoss-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. Burvoss-Carter et al., Phys. Rev. Lett. 81, 1445 (1998)]. We study the effect of surface segregation. 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 the interface perturbation is predicted to decay under tension and grow under compression. The evolution of rippled interfaces created artificially by lithographic techniques is being studied by optical interferometry and cross-section STEM. The results are compared to theoretical predictions and to previous experiments. Implications are discussed for the kinetics of shanking during growth from the vapor.

3:30 PM 14.5

Morphological and Compositional Instabilities of Strained and Unstrained Alloy Layers - Theory and Experiments. Frank Gill, Grame-Telecom, CNRS, 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 can produce an instability if the strain parameters (temperature and wavenumber) associated with the modulation are critical with respect to each instability. In the case of lattice-matched layers, the proper morphological instability disappears. However, Transmission Electron Microscopy (TEM) and X-ray micromodulation 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 depends by bunching of the modulations layer superlattices was systematically studied. Growth of both tensile and compressive layers on surfaces variously oriented with respect to [001] allowed us to investigate two debated questions. Does the morphological instability depend by bunching of the modulations, or is there nucleation of new steps? What is the nature of the symmetry between tensile and compressive layers? The main result is that, in these experiments at least, for layers under compression, the surface nonuniformity 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 14.6

Steady-State Structures in Composition-Modulated Alloys: Kinetic Phase Transition between 1D and 2D Patterns. Vitaly 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 nucleate 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 alloy by growing alloy and present 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 zinc-blend semiconductors and show that the steady-state structure is governed 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 90° system, and a 2D pattern is a square one. In the latter, alloy composition is modulated in [100] and [001] directions, whereas surface undulations occur in [110] and [110] directions. Surface diffusion anisotropy favors a rhombohedral rather than the square lattice. We discuss experimental data that reveal 1 kinetic phase transitions between 1D and 2D patterns in InAlAs/InP growth and ii) a nonplanar surface modulated in [110] and [110] directions in GaInAs/GaAs growth. [1] J.E. Guyer and P.W. Voorhees, Phys. Rev. B 54, 11710 (1996). [2] F. Lovon and R.C. Donn, Phys. Rev. B 57, 4805 (1998). [3] I.P. Ipatov, V.G. Malyshkin, A.A. Maradunsky, V.A. Shchukin, and R.F. Wallis, Phys. Rev. B 57, 12968 (1998).

4:15 PM 15.4.7


Quasi-periodic lateral superlattices are formed by spontaneous compositional modulation along the growth front during molecular-beam epitaxy of AIAs-InAs short-period superlattices (SPS) 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 laterally modulated materials. 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 growth conditions are monitored. The degree of compositional modulation and the growth rate of AIAs-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-sublattice exchange model. The Division of Basic Energy Sciences in the Office of Science of the United States Department of Energy (DOE) supported this work under contract.
of growth by diffusion-limited aggregation. At the highest temperature studied (550°C), the dot size distribution narrows as predicted by the thermodynamic argument. Together with the apparent growth of incoherent particles, it is a sign that the growth is transformed from kinetically to thermodynamically driven. Our results indicate that many published results can be reconciled by the scale of growth temperature. We will discuss our results in terms of current models for coherently quantized dot growth. We show that the monatomic surface steps can be used to partition the etch mask area for dot quantization of dot growth. With proper preparation, regular or spotted patterns 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 the dot-doped GaAs quantum dots, the transport properties of the two-dimensional electron system exhibit strong quantum coherence caused by dot alignment.

11:00 AM **E.5**

**NANO-SCALE PROBE ASSISTED SITE-CONTROL OF QUANTUM DOTS WITH NANO-METER PRECISION**

Hisashi Nakamura, Shigeru Kohmoto, Tomonori Ishikawa* and Ryoko Asakawa

The Femtosecond Technology Research Association (FESTA), Tsukuba, Japan

*NEO Industrial Technology Fellowship Researcher

Nano-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 self-assembled QD by use of a UV light patternning multi-channel system. A nano-scale deposition 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 deposition could not as a monolayer, the following GaAs growth formed a nano-scale just above the deposition. Then, 1.1 monolayer InAs supplied produced a QD on the hole electrode which could act as the favorite site for the strained QD. Undesirable Stranski-Krastanov QDs were not observed as an off-site effect. Using this technique, we successfully demonstrated a 100 nm-pitch array of paired 30 nm-diameter-QDs with 1.5 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 NEO within the framework of the Femtosecond Technology Project.

9:15 AM **E.4**

**STRAIN ENGINEERING OF NANOSCALE STRUCTURES IN THE Ge/Si SYSTEM**

Masayoshi Nagahara, University of Wisconsin-Madison, Madison, WI

Many current devices utilize the use of strained semiconductor thin films. Strain engineering can also be used for fabricating three-dimensional nanostructures through nanoscale 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 microscopic as well as patterned Si(001) and SOI(001) surfaces. Using focused ion beam microscopy and low-energy electron microscopy, we characterize surface strain fields and surface/interface structures and morphologies, as well as the strain of films on silicon and growth. The lattice strain induces formation of ordered arrays of three-dimensional islands with reproducible spatial and size uniformity, providing a potentially attractive route to fabricating novel devices involving arrays of quantum dots. We also discuss theoretical analyses and models based on elastic modeling to elucidate the formation and selforganization processes driven by strain relaxation.

10:15 AM **E.5**

**STRUCTURAL AND MORPHOLOGICAL SURFACE EVOLUTION OF LAYERS GROWING UNDER STRAIN**


Understanding the factors affecting surface roughening in heteroepitaxy is equally crucial for obtaining flat high quality epitaxy in planar device technology, and for controlling self-assembly of threedimensional nanostructures. We have investigated the effects of the magnitude and sign of misfit strain on the evolution of surfaces during heteroepitaxial growth by growing Si-Ge alloys with varying Ge content, and metal-semiconductor compounds with a presumably-ordered lattice constant. We observe that the former requires an amount of compressive strain in the Stranski-Krastanov layer, while the latter, e.g., covalent diode, 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 using scanning tunneling microscopy (STM) 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 the substrate instability. 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 colonies can evolve into a vicinal surface 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 E5.6
EVALUATION OF THE STRAIN FIELD INSIDE AND AROUND GROWTH WITH LIGHT DIFFUSION SCATTERING. Thomas Weibach, Martin Schmidbauer, Helmut Raatz, Peter Schnee, Rolf Koehler, Wolfgang Neumann, Holm Kirnse, Michael Rabe, Fritz Henneberger, Institut fuer Physik, Humboldt-Universitaet zu Berlin, Berlin, GERMANY; H. Wawra, Institut fuer Kristallzuechtung, Budower Chinnaue, Berlin, GERMANY.

One of the key parameters of nanocrystal growth 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 is reciprocal, the shape related part of diffuse intensity inversely scales with the size of the island, the evaluation of strain becomes the more difficult the smaller the islands are. This can be roughly characterized by the product of strain (island-host) and size (islands). E.g., for a Ge-island on Si (midsize 5% 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 1.5 nm). In the latter case the results are compared with transmission electron microscopy data.

11:00 AM E5.7
NEW THRESHOLD RELIEF MECHANISMS FOR Ge/Si(100)
COHERENT ISLANDS. Jeff Drucker, Sergio Chariyap, 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 600 deg C for effective Ge coverages between 3.5 and 14.0 monolayers. We find that the mean dome radius increases and the cases of dislocation introduction is delayed with increasing growth temperature. Also, for temperatures greater than 600 deg C, very large but clusters are observed which populate a peak in island size distributions distinct from and between those of huts and domes. For temperatures greater than 550 deg C, we find that large dome clusters may form at a single temperature which may extend well into the Si substrate. Increasing growth temperature reduces the size at which these clusters appear. Cross-sectional energy dispersive x-ray nanoanalysis analysis 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 the size and decreasing presence of dislocation introduction with increasing growth temperature and the existence of very large clusters. A simple atomicistic elastic model is presented which explains this complex alloying behavior. This model is also used to interpret the formation of islands. We find that island 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 E5.8
NUCLEAR-INDUCED INSTABILITY PHENOMENA ON THE ENERGETIC PATHWAY OF SiGe/Si GROWTH. Silke H. Christmann, Michael Becker, Hartmut Becker, and Horst P. Strunk, Universitat Erlangen-Nuernberg, Institut fuer Werkstoffwissenschaften, Lehrstuhl VIII Mikrostrukturierung, Erlangen, GERMANY; H. Wawra, Institut fuer Kristallzuechtung, Berlin, GERMANY.

Using liquid phase epitaxy from Si substrate growth technique that by its nature performs new thermodynamic equilibrium we analyze the morphological transition from two-dimensional growth via rippling to island formaion in the model system Si(001). We use both atomic force microscopy and transmission electron microscopy to analyze shape and size of the three dimensional morphologies. Systematic growth experiments are dependent on growth rate and temperature and melt fraction 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 an island state at different coverages. From a matrix of that type of gradient specimens we determine nucleation energies of islands as dependent of the melt fraction. 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 wavelength and wavelength of the surrounding ripples. While ripples that surround an island are dissolved, the amplitude of ripplse in a critical distance to the island increase and then decrease again with increasing distance to the island.

11:30 AM E5.9

As a consequence of strain relaxation, Ge coherent islands on Si(001) substrate evolve to different shape (aspect ratio) during deposition. By measuring the island size in 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 shape evolution in Ge islands is also discussed.

SESSION 16/7
JOINT SESSION: ATOMIC SCALE STUDIES
Chair: Venkatesh Narayanasami
Wednesday Afternoon, December 1, 1999
Wellesley (M)

1:30 PM EBI/7.1

In the last few years the scanning transmission electron microscopy (STEM) has become capable of forming electron probe of atomic dimensions, as small as 0.18 nm in diameter. This makes 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 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 Li-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 is independent of the space group structure model. It is shown that the Li 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 represent 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 detailed structure of the ordered structures is important to understand their properties. Ordered structures in GaAs, Si, and Ge have been presented. In GaAs, there is a new ordered structure observed, containing a periodic array of nanophase domains with As-Ge ordering of the As and Ge atoms. The (011) phase domain boundaries are along directions parallel to [110] directions and spaced by 0.1 nm for the zincblende structure. In GaAs, ordered domains show As-Ge ordering of As and Ge atoms. The ordered domains show two variants, [111] and [110] ordered domains periodically forming in a specific superlattice resulting in a discontinuity of the angular momentum. The structures of the nanophase domain boundaries, the orientational domain boundary and the interface between two ordered variants are discussed.

This research was sponsored by the U. S. Department of Energy under contract No. DE-AC05-86OR22643 with Lockheed Martin Energy Research Corp.

2:00 PM *E1.2/7.2*
RAPID QUENCH STI CONDENSATION STUDIES OF InAs QUANTUM DOT FORMATION ON GaAs (001). P.-R. Joyce, T. J. Krzywinski, 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 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 to a molecular beam epitaxy (MBE) 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 studies 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 growth in a capped MBE chamber. 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 facets, and the effects of growth rate on the optical properties of QDs.

2:30 PM *E1.3/7.3*
FORMATION MECHANISM OF METAL OXIDE QUANTUM DOTS: THEORETICAL SIMULATION STUDY. Masayuki Kudo, Yasuuki Inaba, Takuya Onoue, Shizuku Takami, Atsuo Miyamoto, Tohoku Univ., Dept. of Materials Chemistry, JAPAN; Masahiko Kawasaki, Tokyo Inst. of Technol., Interdisciplinary Graduate School of Eng., Yokohama, JAPAN; Minoru Yoshimoto, Tokyo Inst. of Tech., Materials and Structures Lab., Yokohama, JAPAN; Hidekazu 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 between the substrate and thin film. This type of epilayer 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 crystallinity of the quantum dots. However, experimentally it is impossible to clarify the formation mechanism of self-organized quantum dots on atomic scale. Hence, in the present study, we employed our crystal growth molecular dynamics simulator MOODY: [1-4] to simulate the formation process of various metal oxide quantum dots on sapphire (011) surface. For example, when we continuously deposited MgO molecules on sapphire (0001) at 1000 K, the formation of MgO quantum dots was observed. The MgO quantum dots on sapphire (0001) has [111] orientation 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 the first simulation study of the formation mechanism of self-organized quantum dots.


4:15 PM *E3.4/7.4*
FORMATION OF COHERENT , n-Si QUANTUM DOT ARRAYS VIA PHASE SEPARATION FROM HOMOGENEOUS ULTRATHIN Sn, Si / / Sn AND Sn, Ge / / Ge EPITAXIAL ALLOY FILMS. Herry A. A. Weezer, Kyu S. Min and Reghin R. J. Thomas, J. W. Morrison Laboratory of Applied Physics, California Institute of Technology, Pasadena, CA.

Diamond cubic α-Si is a direct band gap semiconductor and band structure calculations also predict a direct and tunable energy gap composition range for the α-Si, α-Si, Sn, Ge, Ge alloy systems. One approach for realization of these compounds in semiconductors is to use Si or Ge, where the enthalpy of mixing is highly positive. First, epitaxially stabilized homogeneous Sn, Si, and Sn, Ge,Sn, Ge,Sn, Ge alloys, metastable solid solutions are grown by temperature-modulated molecular beam epitaxy. The α-Si grown homoepitaxial film is then thermally annealed in high vacuum, whereas the Sn grown quantum dots precipitate as the ultrathin α-Si film phase separates. The quantum dots appear in high-resolution transmission electron micrographs as square-shaped particles with length along <100> direction and the size ranges from 2 to 6 nm. The early stages of phase separation are consistent with a commensurate decomposition and later based on a nucleation and growth mechanism, where a high temperature, Sn, Ge,Sn, Ge,Sn, Ge layer evolution occurs via coarsening. Results of optical characterization, including infrared absorption and photoluminescence, will be related to the kinetics of phase separation.

3:05 PM *E3.5/7.5*
CHARACTERIZING ATOMIC-SCALE COMPOSITION VARIATIONS IN EPITAXIAL III-V MATERIALS WITH CROSS-SECTIONAL SCANNING TRANSMISSION ELECTRON MICROSCOPY. Jeremy D. Steinhilber, John R. Harper, Michael B. Werner, Texas A&M University, Dept. of Physics, College Station, Texas.

Many important issues in the epilayer growth of III-V, InGaAs, and InP semiconductor heterostructures and III-V, InP, GaAs, and InP 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. While the use of cross-sectional scanning transmission electron microscopy (STEM) can be used to address this theme by examining several fundamental material characterization issues and furthering our understanding of heteroepitaxial chemistry, the use of cross-sectional STM has many advantages including its ability to provide real-space visualization of cross-sectional chemical heterogeneity. 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 *E3.6/7.6*
MULTI-METAL SIMULATIONS AT ATOMIC-LEVEL SURFACE STRESSES AND MIGRATION PROCESSES ON InAs, GaAs MESAS. Xiaolin Su, Akihiro Nakano, Sanjay Kodiyalam, Rajiv K. Kalin, Priyam Vashistha, Concurrent Computing Laboratory for Materials Simulations, Dept. of Physics & Astronomy, Department of Computer Science, Louisiana State University, Baton Rouge, LA. Anupam Muralikumar, 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 in-house developed in-house code (QMS) which is based on the local chemical composition. Multiresolution techniques are used to speed up the simulations. InAs/GaAs square mesa with [110] type side walls and InAs/GaAs square mesa with [113] type side walls are studied. Results will be presented for surface atomic...
stress 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, UCSC-USRI, ARO, NASA, PRF, NSF USA-Japan International Grant, and LEQSF.

**SESSION 17: POSTER SESSION:**
ORDERING/COMPOSITION MODULATION / 3-D ISLANDING
Chair: David M. Pletcher and Angelo Mascarenhas
Wednesday Evening, December 1, 1999
8:00 P.M.
Exhibition Hall D [H]

**P.1**
COMPOSITION AND THICKNESS EFFECTS ON ATOMIC ORDERING IN THE GALLIUM-INDIUM-PHOSPHIDE EPITAXIAL LAYERS. O. Golubin, Emil Zolotovskii, Yigal Komech, Technion-ITI, Dept. of Materials Engineering, Haifa, ISRAEL

GaP-B-type ordering is observed in the GaIn_{1−x}P system for different thicknesses. However, the mechanism of ordered phase formation 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 GaIn_{1−x}P layers (0.47 < x < 0.54) MOCVD grown on GaAs substrates 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 proportional to the duration of growth, and thus in thicker layers the ordering effect should be more pronounced. Epitaxial layers of GaIn_{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 data is needed 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 Δx = 0.0015. As a result, we were able to derive the degree of ordering, η(x), as a function of the layer composition, x, in the close vicinity of x = 0.5, which composition favors complete ordering, η = 1. The η(x)-dependencies exhibited bell-like shapes with parameters determined in the sample thickness range. With increase in the thickness, the bellshaped η(x)-curves were found to be broadened, their maximum values to be reduced and the position of the maxima to be shifted from expected x = 0.5 to x = x_m ≈ 0.516. The latter composition corresponds to the complete matching of the GaIn_{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.

**P.2**

We examine GaP-B atomic sublattice ordering in GaAs_{1−x}P [GaP:B] and GaAs_{1−y}In_{y}As [GaAs:HIVL] 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 by transmission electron microscopy (TEM). Relatively thick (0.5-2.0 μm) double-variant ordered GaP and GaAs films show complementary superdomain formation. Single-variant ordered films (0.15-0.2μm) show single-phase domains, separated by antiphase boundaries (APBs). The appearance of APBs in TEM dark-field images is anticipated from electron diffraction studies.

**P.3**
SINGLE AND DOUBLE VARIANTS GaP-B ORDERED GaAs. R.L. Ferrant, 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 GaAs 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 induced. HRXRD provides an independent means to quantify the order parameter of semiconductor heterostructures on different (111)B symmetric substrates, 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 nearly 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 exactly (001) InP substrates, with an ordering parameter of about 0.1 in both substrates. For substrates which were miscut by 6 degrees, only single variant ordering was detected. In these cases, an order parameter as high as 0.38 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.

**17.4**

It is known that GaP ordering occurs only in the two [111]B directions in GaP alloys. When the GaP epilayer is grown on an exact (001) or [111]B-type GaAs substrate, the two ordered variants are equally favorable and so, ordered domain twins appear in ordered GaP 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 GaP 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. 99, 98 (1998).

**17.5**
LOCAL ORDER OF TE IMPURITY ATOMS IN HEAVILY DOPED GaAs AND ACCOMPANYING ELECTRON LOCALISATION EFFECT. T. Shigemitsu*, E. Zielinski-Rohaczynski, Inst. of Experimental Physics, Warsaw University, Warsaw, POLAND; *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 = 10²⁵ cm⁻³ the free electron concentration can be reversible changed between low value (n < Te) and high one n ≈ 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 Kronig-Penrose 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 localization 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 temperatures. Model of the structure of GaAs:Te solid solution with local order will be supported by below results. Our results indicate that due to an evidence of structural changes of critical character and an arising of long range fluctuations accompanying electron localization 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 existence of chemically bonded dimers of impurity atoms, formulated during last years in the literature and propose electron energy dependent mechanism of their creation.

**17.6**
A-TYPE ORDERING IN AlGaIn_{0.5}As GROWN BY METALORGANIC-VAPOR-PHASE EPITAXY. Tetsu Suzuki, Opto-Electronic Device High-Frequency Research Center, NEC Corp., Toshiro Ishibashi, Fundamental Res. Labs., NEC Corp., Masayoshi
Triple-Period-A (TPA) and CuPt-A type ordering as well as conventional CuPt-B type ordering have been observed in III-V semiconductor alloys grown on (011) III-V substrates by molecular beam epitaxy (MBE). Surface reconstruction during growth, which for these types of ordering are (2×3), (1×2) and (2×2), respectively. These relations definitively established the responsibility of surface re-constructions during growth to ordering on a substrate. In turn, for the growth of CuPt-B type ordering, the metallography of vapor-phase epitaxially (MOVPE) grown III-V semiconductor alloys indicate the existence of (2×2) reconstruction during these III-V growth. This leads to the question whether A-type ordering such as TPA 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 TPA and CuPt-A type ordering in Al$_x$In$_{1-x}$As grown by MOVPE at a low temperature of 300°C. This indicates that the metal structures of (2×3) and (1×2) exist in this alloy during growth even in MOVPE when growth temperatures are low.

17.7 USE OF MISCELLANEOUS TO EXTEND LATERAL COMPOSITION MODULATIONS IN InAs/AlAs SUPERLATTICES: John L. Ruoff, David Y. Boulton, Stephen R. Lee and Eric D. Jones, Sandia National Laboratories, Albuquerque, NM. Andrew G. Norman, Scott P. Ahrenkelt, Helio R. Moutinho and Angelo Mascarenhas, National Renewable Energy Laboratory, Golden, CO.

The microstructure of composition modulation in [In$_{m}$As$_{n}$]/[Al$_{m}$As$_{n}$] short-period superlattices grown on (001) InP has been well characterized. For optimum growth conditions [n = 0.5 - 2.0, T$_{m}$ = 550°C] only complete modulation of In$_{m}$As$_{n}$ growth was observed in one direction with only short extension in the growth plane (n > 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 [30] and [31]. We have also found that the composition variations produced in these alloys are quite large: local enrichments in In concentration up to In$_{10}$As$_{90}$ have been determined. With the intent of producing extended modulation in the growth plane that are along one direction only, we are examining growth on miscut substrates. We have grown superlattices with n = 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 preferred [331] and [311] 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 towards (011), the modulation has one predominant direction. Furthermore, the modulation extends 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 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 plane regions.

17.8 PROFILING COMPOSITION VARIATIONS IN COMPOSITION-MODULATED GaP-InP SHORT-PERIOD SUPERLATTICES USING RESONANCE RAMAN SCATTERING: Hyunsik M. Cheong, Yong Zheng, A. G. Norman, J. D. Perkins and A. Mascarenhas, National Renewable Energy Laboratory, Golden, CO.

We use Resonance Raman scattering and electron energy loss spectroscopy to profile the composition and strain variations in laterally composition modulated GaP-InP short-period superlattices. The electron energy loss spectrum of a GaP$_{20}$/InP$_{30}$ short-period superlattice gives the fundamental band gap energy of the InP superlattice at 1.62 eV, which is about 20 meV lower than the band gap energy of a GaP 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 excitation. On the other hand, when the polarizations are orthogonal to the composition modulation, the LO phonon redshift as much as 16 cm$^{-1}$ at low excitation energy. A comparison of the experimental data with a model calculation gives the average In composition in each layer as 0.7% and the maximum InGa composition in the GaP-rich region as 0.8% ± 0.02. Our result also indicates that there are small volumes (less than 1% volume fraction) with very high In mole fraction.

17.9 RECIPROCAL SPACE X-RAY MAPPING AND TRANSMISSION ELECTRON MICROSCOPIC STUDIES OF COINCIDED InAs AND CUBIC CLUSTER SUPERLATTICES IN GaAs FILMS GROWN BY MOLECULAR-BEAM EPITAXY AT LOW TEMPERATURE: V. V. Chalyshnev, N. A. Bert, N. N. Faleev, Yu. G. Muskin, A. E. Kuniyan, A. T. Tolle Physical Institute, St. Petersburg, Russia, M. V. Prokhorov, E. P. Putyato, E. R. Semenov Institute of Semiconductor Physics, Novosibirsk, Russia; P. Werner, Max-Planck-Institute of Microstructure Physics, Halle, Germany; Y. Takeh, 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 strain-modulation or in the film bulk due to precipitation a saturated 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 inserts 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 we employed to assess the crystalline quality and parameters of both InAs and A-cluster superlattices. The nanograin InAs/GaAs superlattices were found to be very perfect in spite of the high (10$^{15}$ cm$^{-3}$) concentration of excess-arsenic-like 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 accommodation of the great majority of the clusters in a multiperiodic regular superlattice.


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.

17.11 THERMODYNAMIC STABILITY OF LATERALLY COMPOSITION-MODULATED PHASES IN ULTRATHIN SURFACE ALLOY FILMS: Yukitoshi Okawara, 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(k). In pseudomorphic ultrathin surface alloys V(k) is proportional to -k$^4$ at the origin, thereby guaranteeing a minimum at k ≠ 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.

17.12 TEM INVESTIGATION OF SELF-ORGANIZED PS-QUANTUM DOTS AS A FUNCTION OF THEIR LAYER LATTICE MATCH AND GROWTH TEMPERATURE: H. H. Kang, L. Subhmanee-Riba, Materials and Nuclear Engineering Department, University of Maryland, College Park, MD; M. Pinczóth, G. Springholz, G. Bauer, Institute for Halbleiterphysik, University of Linz, Altenbergersstr, Linz, Austria.

The study of the morphology, lateral, and vertical correlation of self-organized PS-quantum dots in PbTe is presented. The samples consist of quantum dot superlattices of n periods of
17.13 TRANSMISSION ELECTRON MICROSCOPY INVESTIGATION OF THE MORPHOLOGY AND THE COMPOSITION OF InGaAs quantum dots. Xiaohou Liu, Jing Zhou, David J.H. Cockayne, The University of Sydney, Australia; Key Centre for Microscopy and Microanalysis, Sydney, NSW, Australia; Rosal 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 InGaAs quantum dots (QDs) have been investigated using transmission electron microscopy. The side profiles of the quantum dots are imaged with a continuous tilting experiment of cross-section specimens which are all well shaped with constant base protrusions. Unambiguously show that the unburied dots are well shaped with circular bases. Significant differences in the image features of the unburied QDs grown on (001) and vicinal (001) GaAs were seen on [011] on-axis bright-field images. Simultaneous images were obtained by modeling the strain field distribution of the QDs with finite element analysis and then using this model to interpret the 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 images of the unburied QDs grown on (001) and vicinal (001) GaAs were seen on [011] on-axis bright-field images. Simultaneous images show a square contrast that suggests a QD morphology with four edges parallel to <100>. The simulated image, however, suggests that a buried InGaAs QD with a circular base can produce a square-shaped image. These observations lead to the conclusion that the buried QDs are also well shaped.

17.14 STRUCTURE OF INAs INCLUSIONS IN Si MATRIX. Nikolai D. Zakharov, Peter Werner, Msc-Phanik Institute of Microstructure Physics, Haller/Snade, Germany; Robert Heitz, Dieter Bieckert, Technical University of Dresden, Germany; minced N. Zakharov, Victor M. Ustian, Dmitri V. Deriev, Boris V. Volovik, Zhores I. Alferov, A.F. Ioffe Physics-Technical Institute, St. Petersburg, Russia; George E. Cirin, 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 technology was shown to 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 characteristic hexagonal shapes with high photoluminescence efficiency a new type of InAs inclusions was found. They are defect free, have zigzag shape with periodicity 1.5 nm and a size close to 1.05×1.3 nm. The absence of misfit dislocations indicates that they are coherently fit to the Si matrix and that their volume is well below thecritical one.

17.15 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 vertical and multi layer mono-shell of the InGaAs on the GaAs (001) surface. The density of QDs increases rapidly from ~110/μm² (at a total deposition of 4 ML deposition) to ~270/μm² (at 5 ML) and saturates at this level up to 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 (≤ 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 suggest that the transition 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.

17.16 THERMAL INDUCED FORMATION OF SILICON ISLANDS FROM SILICON ON OXIDE SUBSTRATES. Bernard Legrand, Vincent Agnese, Vincent Sene, Didier Stevermer, IEMN, Villeneuve d'Ascq, France.

Starting from SOI substrates with 3 to 20 nm thick silicon layers, we show how silicon islands can be reproducibly generated in UHV in the 850-975°C range for a few minutes. The temperature evolution 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 ranges from 10 to 100 nm (depending on the temperature, (<100°C)>). GaAs 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.

17.17 NANO-STRUCTURAL INVESTIGATION OF InAs QUANTUM DOTS MULTI-STACKED ON GaAs (100) SUBSTRATES. Cheong Hyan Rho, Seon Woo Lee, Kwang Bo Shim, Hangeun 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 thickness of the GaAs spacer and the InAs wetting layer were 5.7 nm and 1.86 ML, respectively. The microstructural 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 a-wafer-like defects were vertically formed along the growth direction of the InAs stacking layers greater than 10 periods. Especially, in case of InAs stacking layers with 10 and 15 periods, the vertically columned InAs QDs grew in parallel with the growth direction of the wafer-like defects. The highest PL intensity was obtained from the specimen with 3 stacking layers and the energy of the PL peak was slightly increasing with stacking layer. The origin of the splitting phenomena was estimated by the temperature-dependent PL measurement.

17.18 THE GROWTH OF InAs SELF-ASSEMBLED QUANTUM DOTS ON InGaAs/InP BY METAL-ORGANIC CHEMICAL VAPOR DEPOSITION. Hyunsik Ason, Sukho Yoon, Tae-Wan Lee, Youngbok Moon, Heesun Hong and Eunyong 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; Hyeon-Seok 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) or quantum well (SQW) are necessary for the realization of next-generation, high-performance optoelectronic devices. Various dot/substrate combinations such as InGaAs/InP, InP/GaAs, InAs/GaAs, InAs/GaAs, InAs/GaAs Al/InP, and InAs/InP have been explored. Among these, the InAs/GaAs Al/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/GaAs Al/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/InGaAs/InP quantum dots on InP substrates with and without growth interruption, and the optical properties were studied by photoluminescence (PL). The average lateral dimensions of uncapped InAs QD growth on a 3 ML InAs/InP multilayer was 60 nm, while the average height range was 9.5 nm. We obtained high-quality InAs/InP quantum dots with a maximum height of 2.5 nm. We also observed high-quality InAs QD growth on a 3 ML InAs/InP multilayer, and the average height range was 9.5 nm, while the average height range was 9.5 nm. We obtained high-quality InAs/InP quantum dots with a maximum height of 2.5 nm. We also observed high-quality InAs QD growth on a 3 ML InAs/InP multilayer, and the average height range was 9.5 nm, while the average height range was 9.5 nm. We obtained high-quality InAs/InP quantum dots with a maximum height of 2.5 nm. We also observed high-quality InAs QD growth on a 3 ML InAs/InP multilayer, and the average height range was 9.5 nm, while the average height range was 9.5 nm.

17.10 THEORETICAL STUDY ON THE EFFECT OF MISFIT DISLOCATIONS ON THE FORMATION OF InAs QUANTUM DOTS ON GaAs SUBSTRATES. Norihito Oyamada, Eiji Ohno, Keio Univ., Dept. of Applied Physics and Photon-Information, Yokohama, Kanagawa, JAPAN.[2] Keiko Ootsuki, Kyoto University, Dept. of Material Science and Engineering, Kyoto University, Toyokawa, Japan, and Institute of Electrochemistry, National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, JAPAN.

It has been reported that the growth mode of InAs/InP strongly depends on the substrate orientation.[2] On a GaAs(001) substrate, the growth mode of InAs epilayers is Strakas-Kratzean 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 microstructural misfits at the dislocations generated at the InAs/GaAs(110) heterointerface by using the first-principles calculations. We found that the dislocation core has a symmetric free-standing conduction band. Such screw dislocations have been previously observed in pure crystals. However, the core structure does not contain unfavorable bonds (As-As and Ga-Ga bonds), it is easy to generate the screw dislocations during the initial stage of epitaxy. Accordingly, the growth mode of an InAs epilayer becomes two-dimensional in the presence of misfit dislocations. This type of dislocation is also possible at InAs/GaAs[111]A interfaces from the geometrical viewpoint. Therefore, it is expected that the growth mode of an InAs epilayer on a GaAs(001) substrate is also two-dimensional. On the other hand, screw 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 dislocation structure (a non-locatable bond structure for 5 and 7 dislocations). Because the generation of 5 and 7 dislocations is restricted by the unfavorable structure, the growth mode on the (001) substrate becomes Strakas-Kratzean 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 screw dislocations is impossible.[1] J. G. Belk et al., Phys. Rev. Lett. 78, 475 (1997).[2] H. Yamaguchi et al., Phys. Rev. B55, 1357 (1997).

17.20 SELF-ORGANIZATION, SHAPE TRANSITION AND STABILITY OF EPITAXIAL STRAINED ISLANDS. X. Wang, Z. H. Zhang, M. R. Bao, National University of Singapore, SINGAPORE.

Strain-induced self-organization of epitaxial islands has been considered of great interest 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 mismatch are taken into account. It is found that the phenomenon 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 mismatch. By linking the surface energy mismatch to the change of the annealing temperature and the change of the materials composition, the inconsistencies that exist in the experiments can be explained. Moreover, the present simulations predict that if we can choose the surface energy mismatching the material properties and/or by changing the annealing temperature, then the strongly self-organized and non-ripening island arrays can be obtained.

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

One existing 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 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 dots in a 1.0 monolayer InAs wetting layer on a GaAs substrate is known to aggregate into quantum dots due to a inherent strain 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 those quantum dots are lens-shaped when embedded in GaAs. Although the effect of coherency strains in causing self-organization 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. However, the generation of self-organized quantum dots can be studied 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 strain will also be illustrated in the calculations. The results of the calculations will be compared with the data available on the experimental measurements of strains.

17.22 THEORETICAL STUDY ON MISFIT DISLOCATIONS IN SELF-ASSEMBLED GaSb QUANTUM DOTS ON GaAs[001] SURFACES. Ko Okajima, Kyusyu University, Dept. of Materials Science and Engineering, Kyushu University, Toyokawa, Japan, and Institute of Electrochemistry, National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, JAPAN.

It has been reported that the GaSb self-assembled quantum dots on GaAs[001] substrates are formed during the initial heteroeptaxial stage 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 deeper insight and understanding, we carried out on GaSb on GaAs[001] a first-principles calculation. 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 growth mode can be explained by a self-organized quantum dots. We also investigated these misfit dislocations microscopically by using first-principles calculations. Using first-principle geometrical optimization, we found a 5x7 membered ring (M) structure at the dislocation core. This structure was formed by the elongated commensurate (Ga-Ga) or non-commensurate (As-As) weak bonds. These weak bonds appeared on both GaSb and As-terminated surfaces, resulting in the formation of similar 5x7 M structure on both surfaces. We also investigated square arrays of misfit dislocations at this interface and found that the results were compared with those of the InAs/GaAs[001] system.

17.23 STRUCTURAL AND OPTICAL PROPERTIES OF SELF-ORGANIZED QDS IN InAs/Ga0.55Al0.45As MULTILAYERS ON (001) InP GROWN BY MOLECULAR BEAM EPITAXY. Z. Zhang, Z. Sun, J. Wu, X. Peng, X. Liu, X. Yang, Z. Chen, X. Jin, Y. Ye, W. Zou, Q. Li, Y. Li, T. Xia, D. Liang, Z. Wang, L. 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/Ga0.55Al0.45As quantum dots on InP substrate was demonstrated for the first time. The samples were grown by a 5-her 3D MBE system. After oxide desorption, deposition of a 0.2 nm InAs seed layer, followed by the growth of 5 bilayers, in which InAs QD layer with
certain nominal thickness were separated by 1.1 nm In$_{0.52}$Al$_{0.48}$As spacer layer. The effective thickness of InAs was 1.9 nm in the present work. The structure was deposited by a 7 nm In$_{0.52}$Al$_{0.48}$As layer. Growth interchanges of 20 s were used at both In$_{0.52}$Al$_{0.48}$As and InAs heterointerfaces. The growth rates of InGaAs and InAs were ~0.76 and ~0.41 μm/h, respectively. Arsenic vapor pressure used in growth was approximately (8°) $10^{-6}$ Torr and the growth temperature was 510°C.

The structural and optical properties were characterized using x-ray diffraction, TEM, and PL, respectively. In the TEM image, the coherent dots were evident through the characteristic dark/white contrast related to different material composition. It was estimated that the average height and lateral size of dots was 3.6 and 2.8 nm, respectively, and the value of height-to-lateral size was between 0.15 and 2.0. In PPL measurements, narrow emission withFWHM of 200 μm was achieved from QDs multilayer structure, which shows the potential for further optoelectronic application.

**17. 24**

**SURFACE PHOTOCHEMISTRY MONITORING OF InAs/InP QUANTUM DOT FORMATION:** Shin-Kyeong, Heedon Hwang, Yon-Wei Lee, Young-Joo Moon, and Yeong-Gun Yoon, School of Materials Science and Engineering, Seoul National University, Seoul, KOREA; Yong-Dong Kim, Department of Physics, Kyung Hee University, Seoul, KOREA; Uk Hyun Lee and Donghan Lee, Department of Physics, Chonnam National University, Gwangju, KOREA.

The self-assembled quantum dot (SAQ) 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 (RHEED) has been used to monitor the 2D-3D transition. However, the high-pressure environment of metalorganic chemical vapor deposition (MOCVD) precludes the use of RHEED. To study the InAs quantum dot formation during growth interruption (GI) or different atmospheres, 3-monolayer-thick InAs layers were grown at 550°C on InP by MOCVD, and subsequently the 30-s GI was provided at different atmospheres of As$_2$/H$_2$/PH$_3$/H$_2$ before the InP capping layer was grown. 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 As$_2$/H$_2$ atmosphere, the SPA signal increased initially and then saturated. It did not change at H$_2$/PH$_3$ atmosphere and it, on the contrary, slightly decreased at PH$_3$$_2$/H$_2$ atmosphere. The samples grown at As$_2$/H$_2$ atmosphere showed a QD photoluminescence (PL) peak at 0.77 eV, whereas those of the H$_2$ and PH$_3$/H$_2$-treated samples showed only PL peaks from thick InAs quantum well with monolayer thickness fluctuation, judging from the energy bandgap of the InAs quantum well. 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.

**17. 25**

**TEX AND PL STUDIES OF INAs AND In$_{0.52}$Al$_{0.48}$As SELF-ASSEMBLED QUANTUM DOTS ON InP SURFACE-REACTED.** Zhongzhe Sun, Ji Wu, Fengqi Liu, Huina-Zhe Xu, Yongli Chen, Xiaoying Ye, Weihong Jiang, Bo Xu, Zhong-gao Wang, Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, Beijing, P.R. CHINA.

In this paper, In$_{0.52}$Ga$_{0.48}$As, In$_{0.52}$Al$_{0.48}$As and InAs self-assembled quantum dots (QD) are grown by Strasnick-Krammers growth mode on In$_{0.52}$Ga$_{0.48}$As passive-matched to (001) InP substrates by a Riber 3SP MBE system. The structural and optical properties were characterized using TEM and PL, respectively. Experimental results reveal obvious effect of etch topology on QD formation, size distribution and luminescence. Due to reduction of strain in ternary In$_{0.52}$Ga$_{0.48}$As, In$_{0.52}$Al$_{0.48}$As layer, they show larger critical thickness for quantum dots formation than InAs layer. TEM results show ternary In$_{0.52}$Ga$_{0.48}$Al$_{0.48}$As dots have relatively larger size (400 nm and 800 nm) than InAs dots (34 nm). In addition, In$_{0.52}$Al$_{0.48}$As dots show larger size, lower density than In$_{0.52}$Ga$_{0.48}$As dots. PL results show relatively strong quantum dots luminescence at around 0.670.78 eV, the FWHM of the intensity of In$_{0.52}$Ga$_{0.48}$As and InAs dots are 39, 67 and 142 meV, respectively. We attribute the narrow emission linewidth from ternary QDs to low sensitivity of QD ensemble with larger size for size fluctuation. The linewidth from In$_{0.52}$Ga$_{0.48}$As is narrower than In$_{0.52}$Al$_{0.48}$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.

**17. 26**

**PHOTOREFLECTANCE INVESTIGATION OF InAs/GaAs SELF-ASSEMBLED QUANTUM DOTS GROWN BY ALMBE.** Massimo Gatteschi, Carlo Raffaelli, Giorgio Guizzetti, Maddalena Patirni, Francesco Pianin, Dept. of Physics, Parma, ITALY; Secondo Branci, Paolo Frigeri, CNR-MASPIC Institute, Parma, ITALY.

Although the optical properties of InAs quantum dots (QDs) have been extensively investigated by photocurrent 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 dot arrays grown by Atomic Layer Molecular Beam Epitaxy (ALMBE). The samples consist of N planes (N=1 to 9) of InAs self-assembled quantum dot layers (SAD), 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 1 nm thick GaAs layers. [1] Photoreflectance measurements have been performed in the 0.8-1.5 eV energy range. The optical properties of the QDs 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 ~1 eV with a transition broadening of ~30-50 meV and an exhibited temperature behavior similar to the InAs structure. A peak at ~0.7 eV, which increased from 1 to 2 eV, was observed in all samples with a significant blueshift (~30 meV) of the SAD PR features; on the other hand a weak redshift (~5 meV) with 30% reduction of the transition broadening appeared with successive layers (N>1) were added. In the case of the ground state transition energy vs. the number of stacked layers of the combined effects of vertical coupling and Coulomb interaction and evidence is given to the possibility of an optical charactristics and quantum dot heterostructures, even at room temperature, taking advantage of the derivative-like nature of PR technique. [1] P. Frigeri et al. J. Crystal Growth n press. [2] L. Aigouy et al. Appl. Phys. Lett. 70, 3329 (1997)

**17. 27**

**NANO-PHOTOLUMINESCENCE STUDIES OF SELF-ASSEMBLED QUANTUM DOTS.** H. Hocon, Hongbin Yu, D. Kulk, J. Ketao and C.K. Shui, O. Bakkenes and A.L. Holmes, Jr. 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 because their mechanical and electrical properties are not shared by other quantum dot structures. In atomic physics, QDs have no counterparts 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 single QD from that of an ensemble. By using nano-aperture method and cross-section enhancement, 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 derivative-like nature of PR technique. We have thus successfully used a PR to study the PL of QDs in nano-meter scale: Inter-dot Carrier Shuffling and Multiparticle States' Submitted to Phys. Rev. B.

**17. 28**

**ELECTRICAL PROPERTY OF NANO SCALE TiSi$_{2}$ ISLANDS ON Si.** Jun-Hee Chai, Hoon Hyeon, Peter Lakki and R.J. Nemethic, Department of Physics, Northern 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 (~110°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 showed a different conductivity between islands and substrate as the bias was 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 high biases, the I-V spectra shows negative differential resistance (NDR). These effect can be explained in terms of the leakage current between the island and substrate and the tunnel junction.
17.30

**FABRICATION OF EPITAXIAL PYRAMIDAL ISLANDS ON Ge(100) USING Sn/C LITHOGRAPHIC MASKS.** Jie Zhang, Douglas J. Swanson, 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 last decade, these islands typically observed during coherent strained layer epitaxy, these models 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 the 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 layer. Additional evidence for the unique islanding mechanism is discussed, along with more detailed description of the changes in film morphology with variation in growth conditions.

17.31

**STRAIN RELAXATION AND 3-D CLUSTERING OF HETEROEPITAXIAL SiGe FILMS VIA STRESS-DRIVEN SURFACE EVOLUTION.** Connie S. Qiu, Aken, 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 stress-free SiGe 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.

17.32

**MOIRÉ PHASE EFFECTS OF THE SIGN OF THE MISFIT STRAIN.** B.G. Demczyk, U.S. Air Force Research Laboratory, SNH, Hanscom AFB, MA. A.H. King and R.J. Guinbalo, 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 filmsubstrate misfit strain, systems tend to minimize (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 partially amorphous Ge films, or those prone to the formation of surface undulations, while films in tension are more heavily defected. These results are discussed in light of the mechanics of dislocation formation in semiconductor structures.

17.33

**PULSED MAGNETIC FIELD INDUCED 3-D ISLANDING OF OXYGEN CONTAINED CLUSTERS IN Ga-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) clusters [like-structures in silicon crystals grown by Czochralski method (Cz-Si)] was investigated [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 supercritical 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 Si₃O₄V, complexes. The PMF-induced microstructure evolution culminates in the formation of spatially ordered oxygen-vacancy clusters and for the oxide precipitates, depending on the oxygen defects present in the crystal. STM and SE studies of the surface topology of the Cz-Si crystals with layer-by-layer etching showed that PMF-induced effects are 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 is a result of 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 Si₃O₄V, clusters emit light in the green region of spectrum under the UV laser excitation. 1. M.N. Levin, B.A. Zon, MSRS Spring Meet. Abstr., G2.9, 1999.
and low energy electron microscopy. The Ge/Si(001) system is of great interest because of the existence of two island shapes, shallow pyramidals and deep convex domes that form when the growth is performed at low temperatures. Low energy 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 develop 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 facets. These asymmetric transition states 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: the inclusion of one transition state (pyramidal to 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 #8/2/NO.2 EPITAXIAL GROWTH OF GERMANIUM ON Si(001) - STUDIES BY HIGH TEMPERATURE STM DURING GROWTH. Bert Voigtländer and Martin Kastner, Institut für Festkörperforschung und Vakuumphysik, Forschungszentrum Julich, GERMANY.

We use a scanning tunneling microscope (STM) capable of imaging the growing layers 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(001). The periodicity of the (2\times2) 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 (2\times2) reconstruction to the Si(001) reconstruction temperature and Si/Ge intermixing. A quantitative comparison to total energy calculations predicting the periodicity of the (2\times2) reconstruction with the experimental results is used to estimate the amount of Si intermixing. The energy barrier for the repeated growth of a new atomic layer on the Ge islands is measured by the growth of a new layer on the islands. This behavior is explained by self-limiting growth. A kinetic growth model involving a nucleation barrier for each repeated growth of a new atomic layer on the Ge islands agrees with the experimental results for the evolution of the island volume, and additionally the shape transition from the previously observed square shape transition to 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 #8/3/NO.3 CHEMICAL ORDERING AT AND NEAR SURFACES: A UNIQUE INPUT OF GRAZING INCIDENCE X-RAY DIFFRACTION. Michel Savage-Simkin, LURE, Orsay, FRANCE and Laboratoire de Mécanique et Géotechnique, Orsay, 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 modelled as a function of thermodynamic and kinetic parameters. However, the influence of reconstructions possibly stabilizing a given surface composition has not been introduced into the model. We consider the particular case of III-V semiconductor ternary alloys (In,Ga)As on GaAs(001), specific commensurate 2\times3 or incommensurate 2m (2.5\sqrt{2}\times3) 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 us to ascribe the 2\times3 reconstruction to a chemically ordered distribution of cations in the different subsurface sites defined by the arsenic arrangement. In the incommensurate 2m, with In on the Ga atoms and As on the In atoms, the In composition was thus found located at the value In 0.67Ga-0.33As with a minimal strain in the surface In-As and Ga-As bonds. Incommensurate 2m surfaces could be produced by forcing the indium surface concentration of out of the nominal value and it will be shown that a full account of the difference phenomenon is obtained by considering, in a diffuse scattering formalism, a probabilistic distribution of either indium depleted or indium enriched faults in the 2\times3 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 a series of intermixed ternary (Ga,In)As grown on GaAs(001) will be reported. The studies of the In$_{0.53}$Ga$_{0.47}$As adopted 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 arrangement in the early stages of heteroepitaxial growth and to complement the information derived from local probes such as scanning tunneling microscopy.


Stress plays a critical role in determining the evolution and the properties of heteroeipitaxial 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 extensively 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 film grows pseudomorphically over a much larger region of metastability before relaxing rapidly. In addition, we find that relaxation occurs without additional growth above a critical 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-AC04-94AL85000.


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(001) and the faceting of vicinal surfaces during metalorganic chemical vapor deposition (MOCVD). We have observed transitions between the classical homoeopitaxial growth modes (step-flow, layer-by-layer, and three-dimensional) as a function of growth rate and temperature on singular GaN(001) 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-ordered [1].

11:15 AM #8/6/NO.6 DAVID TURNBULL AWARD LECTURE ATOMIC-LEVEL CONTROL DURING FILM GROWTH UNDER HIGHLY CONCENTRATED AND ULTRA-HIGH-DOPING IN Si$_{1-x}$Ge$_x$ GAS-SOURCE MBE. J.E. Greene, Univ of Illinois-Urbana, Materials Science Dept and MDA, 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$_2$H$_6$/Ge$_2$H$_4$ mixtures have been investigated using a combination of in-situ RHEED, EELS, STM, 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 D₂ 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 sp² 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.