SYMPOSIUM N

Atomic Scale Measurements and Atomistic Models of Epitaxial Growth and Lithography

November 30 – December 2, 1999

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* Invited paper

8:30 AM *N1.1
EFFECTS OF INTERFACE ROUGHNESS AND
MICROSTRUCTURES ON DEVICE TRANSPORT PROPERTIES.
David Z.-Y. Ting, Jet Propulsion Laboratory California Institute of
Technology Pasadena, CA.

A three-dimensional quantum mechanical scattering calculation is
used to analyze the effect of interface roughness and microstructures
on device transport properties. The following topics will be discussed:
(1) effect of interface roughness on resonant tunneling in double
barrier structures,
(2) resonant tunnelling via InAs self-organized quantum dot states,
(3) effect of interface roughness on the tunneling characteristics of
ultrathin oxides, and,
(4) embedded quantum wires as a model of dielectric breakdown.

9:00 AM N1.2
MORPHOLOGY CONTROL IN 6.1ÅMBE USING IN-SITU
SENSORS. J.H.G. Owen, W. Barvosa-Carter, Math. Dept. UCLA,
Los Angeles, CA; J.J. Zinck, HRL Laboratories, Malibu, CA.

Aggressive design of high-speed devices based on the 6.1Å family of
III-V materials, InAs, AlSb, GaSb, requires control of the morphology
of critical interfaces within tight tolerances. Growth sensor signatures
- in particular, RHEED and Photoemission (PE) - are sensitive to
growth parameters such as flux, temperature and V/III ratio, all of
which may be utilized for active control during growth. However, the
in-situ sensors do not give direct morphology information. To address
this issue, we have correlated the RHEED and PE data with in-situ
STM of the grown surfaces and used the results to calibrate a Kinetic
Monte Carlo (KMC) model. We are developing a control model based
on this KMC model which will allow us to control surface morphology
during MBE growth.

9:15 AM N1.3
IN SITU SENSING OF MORPHOLOGY BY THRESHOLD
PHOTOEMISSION DURING MBE GROWTH. J.J. Zinck, HRL
Laboratories, Malibu, CA; and J.H.G. Owen, UCLA, Los Angeles, CA.

Photoemission (PE) oscillations have been used to monitor and
control deposition of device layers with submonolayer resolution in a
manner analogous to RHEED oscillations [1]. However, even in the
absence of oscillations, threshold photoemission measured during
growth is observed to have a characteristic signature which contains
both chemical and morphological information. We have investigated
this signature during the MBE growth of the 6.1 Å family of III-V
materials, InAs, AlSb and GaSb, as a function of growth temperature,
growth rate, V/III ratio, excitation wavelength and polarization of the
excitation source. Simultaneous RHEED data have been collected to
allow a comparison between the two techniques. PE samples a larger
surface area than RHEED and will therefore be a more stringent test
of nonuniformity. Growth interrupts of several minutes are necessary
to fully recover PE intensities to pregrowth levels, regardless of
whether the substrate is stationary or rotating at 60 rpm. Such
observations suggest that PE signatures are sensitive to morphologies
on length scales not accessible to RHEED, but important for device
fabrication. [1] J.J. Zinck, D.H. Chow, J.N. Schulman, and H.L.
Dunlap, Appl. Phys. Lett. 68, 1406 (1996).

9:30 AM N1.4
THE IMPORTANCE OF MANY-BODY EFFECTS IN THE
CLUSTERING OF CHARGED Zn DOPANT ATOMS IN GaAs.
Ph. Ebert[1], Tianjiao Zhang[2,3], F. Kluge[1], M. Simon[1], Zhenyu
Zhang[3,2], and K. Urban[1], [1]Institut für Festkörperforschung,
Forschungszentrum Jülich GmbH, Jülich, GERMANY; [2]Department
of Physics, University of Tennessee, Knoxville, TN; [3]Solid State
Division, Oak Ridge National Laboratory, Oak Ridge, TN.

The spatial distribution of negatively charged Zn dopant atoms in
GaAs has been investigated by cross-sectional scanning tunneling
microscopy. At high densities, the dopant atoms exhibit a clear
clustering behavior, suggesting the existence of a possible attractive
interaction in addition to the screened Coulomb repulsion between
two dopants. By analyzing the data through Monte Carlo simulations,
we have extracted the intrinsic screening length at different dopant
densities, and attributed the origin of the effective attraction to
strong many-body effects in the dopant-dopant interactions.

9:45 AM N1.5
MICROSTRUCTURE OF EPITAXIAL $Sr_{n+1}Ti_nO_{3n+1}$ THIN
FILMS OF RUDDLESDEN-POPPER SERIES. W. Tian[1], J.H.

Haeni[2], D.G. Schlom[2], and X.Q. Pan[1]; [1]Department of Materials
Science & Engineering, The University of Michigan, Ann Arbor, MI;
[2]Department of Materials Science & Engineering, Penn State
University, University Park, PA.

The controlled synthesis of homologous oxide crystal systems offers
tremendous potential for tailoring the ferroelectric and dielectric
properties of materials. Using an MBE system with in situ atomic
absorption spectroscopy for precise composition control, we have
grown the first five members of the $Sr_{n+1}Ti_nO_{3n+1}$ (n=1-5)
Ruddlesden-Popper homologous series. Film microstructure and the
atomistic structure of crystal defects and film/substrate interfaces
have been examined using high resolution transmission electron
microscopy (HRTEM) in combination with computer image
simulations. Electron diffraction and HRTEM studies indicate that all
films are single crystal, epitaxially grown on the (001) $SrTiO_3$
substrates along the c-axis. The in-plane orientation relationship
between the films and the substrates is identified to be
$Sr_{n+1}Ti_nO_{3n+1}$-[100] // $SrTiO_3$-[100]. Among these five films,
Sr_2TiO_4, $Sr_3Ti_2O_7$ and $Sr_4Ti_3O_{10}$ thin films are nearly free of
intergrowths, indicating that these three phases may be more stable
than other phases of the $Sr_{n+1}Ti_nO_{3n+1}$ series. HRTEM studies
revealed the existence of a large of number of crystal defects such as
antiphase boundary and stacking faults. Based on quantitative
HRTEM studies, structural models of these defects and the
film/substrate interfaces are determined. The growth mechanisms of
the Ruddlesden-Popper type structures will be discussed.

10:30 AM *N2.1
STM STUDIES OF SEMICONDUCTOR ALLOY LAYER AND
INTERFACE STRUCTURE AT THE ATOMIC SCALE. E.T. Yu and
S.L. Zuo, University of California, San Diego, La Jolla, CA.

The atomic-scale structure of heterojunction interfaces and alloy
layers can exert a pronounced influence on electronic, optical, and
transport properties in semiconductor heterostructure materials and
devices. Cross-sectional scanning tunneling microscopy (STM)
provides unique capabilities for probing compositional and electronic
structure at the atomic scale in III-V compound semiconductor
epitaxial layer structures and devices. We will discuss recent
cross-sectional STM investigations in our laboratory of atomic-scale
interface roughness and its correlation with carrier transport
properties, and of atomic-scale clustering and local ordering in III-V
semiconductor alloy layers, quantum wells, and superlattices.
Particular emphasis will be placed on investigations of mixed-anion
material systems, including arsenide-phosphide, arsenide-antimonide,
and arsenide phosphide-antimonide alloys and heterostructures.

11:00 AM N2.2
NOVEL RECONSTRUCTIONS ON THE AlSb AND GaSb(001)
GROWTH SURFACES. A.S. Bracker, J.C. Culbertson, B.V.
Shanabrook, B.R. Bennett, B.Z. Nosho, and L.J. Whitman, Naval
Research Laboratory, Washington, DC; W. Barvosa-Carter, HRL
Laboratories, Malibu, CA.

Heterostructures involving the 6.1Å family of III-V semiconductors
(InAs, GaSb, and AlSb) are integral components of a number of novel
high-frequency and infrared optoelectronic devices. The structure of
the interfaces in these heterostructures can be critical to device
performance, and device optimization will ultimately require precise
and reproducible control over surface morphology during growth. To
accomplish this level of morphological control, models are being
developed which relate process parameters to surface roughness.
These models require a detailed understanding of the relevant surface
reconstructions and the mechanisms by which epitaxy proceeds. Using
MBE, RHEED, and STM, we have discovered that the structure of
the "1×3" surfaces observed by RHEED on AlSb and GaSb(001) is a
strong function of temperature and Sb flux, and actually includes a
number of distinct (4×3)-like reconstructions. Surprisingly, two of
these structures — including the (4×3) surface observed under our
usual device growth conditions — include *mixed* III+V dimers within
the top layer of the structure (as confirmed by first-principles
theoretical calculations[1]). Unlike mixed dimer structures proposed for
some III-P reconstructions, in these cases each III-group atom (Al or
Ga) resides close to its natural lattice site. This configuration leads to
nucleation and growth mechanisms that are fundamentally different
than for other III-V systems, with important implications for
atomistic modeling of the growth process.
1. H. Kim, N. Modine, and E. Kaxiras, to be published.

11:15 AM N2.3
STABLE RECONSTRUCTIONS OF AlSb (001) SURFACE AND
THE THEORETICAL STM IMAGES. Hanchul Kim, Harvard
University, Div of Engineering and Applied Sciences, Cambridge, MA;
Normand A. Modine, Sandia National Laboratories, Albuquerque,
NM; Efthimios Kaxiras, Harvard University, Dept of Physics,
Cambridge, MA.

Novel surface reconstructions of III-V (001) surface, characterized by
(4×3) symmetry and mixed III-V dimers within the top layer, have
been observed in recent STM experiments (conducted at NRL) on the
MBE grown AlSb (001) surfaces. These reconstructions have also been
observed on GaSb (001) surfaces, which indicates they represent a new
family of reconstructions of III-V (001) surfaces. Understanding the
nature of these reconstructions is important for growth mechanisms,
which will be influenced by their atomic-scale features. In order to
elucidate the atomic structure of the (4×3) reconstructions, we have
used the *ab initio* pseudopotential total energy method to examine the
various atomic models of different surface stoichiometry. The sequence
of thermodynamically stable structures is predicted as a function of
the Sb chemical potential, in agreement with experimental indications
for condition relevant to MBE growth. Finally, to illustrate the
agreement between the theoretical predictions and the experimental
observations, we simulate STM images in constant-current mode and
compare them with the available experimental data.

11:30 AM N2.4
AN IN SITU STM STUDY OF Sb DOPING ON Si EPITAXY.
Glenn G. Jernigan and Phillip E. Thompson, Naval Research
Laboratory, Washington, DC.

We have integrated an STM with a commercial Si MBE system for in
situ examination of device structures grown on full 75 mm wafers to
realize methods for fabricating ideal chemical and electrical interfaces.
The effect of Sb doping on Si epitaxy was investigated for its ability
to act as a surfactant during SiGe growth and for the development of
atomically abrupt p-n tunnel diodes. We will present a description of
the surface morphology which evolves from the co-deposition of Sb
and Si. Si was deposited at 0.1 nm/s concurrent with an Sb flux of 3 x
10^{12} atoms/cm/s onto a 500°C Si (100) substrate for 240 s. Under
these conditions, the surface segregation of Sb results in a complete
monolayer coverage on top of the Si surface. The Sb terminated
surface has a round "dimple" morphology with an RMS roughness
greater than that of Si epitaxy without Sb. A flash to 800°C for one
minute desorbs the Sb monolayer revealing the underlying Si epitaxy.
The Si surface consists of a uniform coverage of small rectangular
islands (2-3 nm by 5-15 nm) of Si dimers and does not contain the
clear S_A and S_B step structure which form during growths without
Sb. An attempt to restore the step structure by annealing for 30
minutes at 800°C caused a coalescence of the islands into a small
terraced surface structure. A high density of square pits are observed,
preventing the terraces from merging and forming long step edges.
The presence of dimples, Si islands, and pits as a function of Sb
doping and Si epitaxy conditions will be discussed. This work was
supported by the ONR.

11:45 AM N2.5
DIRECT MEASUREMENT OF THE DIFFUSION OF Ge DIMERS
ON Si(100). X.R. Qin, B.S. Swartzentruber, M.G. Lagally, University
of Wisconsin-Madison, Madison WI; Sandia National Laboratories,
Albuquerque, NM.

We have performed quantitative measurements of the diffusion of Ge
dimers adsorbed on the Si(100) surface using atom-tracking scanning
tunneling microscopy. The Ge dimers, diffusing on top of dimer rows,
have characteristic dynamic properties that differ from those of
adsorbed Si dimers. At low temperature ($\sim$ 300K), adsorbed Si dimers
rotate at a single lattice site [1,2], while Ge dimers rock between two
buckled configurations. At higher temperatures the Ge dimers, like
the Si dimers, diffuse along the substrate dimer rows. The rocking and
hopping rates of the Ge dimers are measured as a function of
temperature and the electric field applied by the tip during tracking.
The corresponding activation energies are extracted. Potential
implications on the early stage of heteroepitaxy of Ge on Si(100) will
be discussed. [1] Z. Zhang, et al, Phys. Rev. Lett. 74, 3644 (1995) [2]
B.S. Swartzentruber, et al, Phys. Rev. Lett. 77, 2518 (1996)
Research supported by Sandia National Labs (Grant No. AS-1168)
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SESSION N3: GaAs SUBSTRATES
Chair: David Z.-Y. Ting
Tuesday Afternoon, November 30, 1999
Regis (M)

2:00 PM *N3.1
GROWTH OF IRON ON GALLIUM ARSENIDE: THEORY AND
PRACTICE. Steven C. Erwin, Naval Research Laboratory, Center for
Computational Materials Science, Washington, DC.

Ultrathin films of magnetic materials on semiconducting substrates
form the basis for a large class of "spintronic" devices. In such
devices, the features of traditional electronics are augmented by the
unbalanced electron spin due to carriers originating in the magnetic
layers. A substantial amount of experimental research has focused on
films of Fe on GaAs, in part because the lattice mismatch between
their bulk phases is extremely small. While the quality of the films
continues to improve, very little is known about the details of the
growth process, the resulting interface structure, or the influence of
interface morphology on properties relevant to device performance. In
this talk, several aspects of the initial stages of film growth are
investigated using first-principles theoretical methods. The focus will
be on the differences between growth of Fe on As-terminated vs.
Ga-terminated GaAs(001), and on the prospects for growth of GaAs
on Fe substrates.

2:30 PM N3.2
CLUSTER MODEL STUDY OF THE INCORPORATION OF
ARSENIC INTO AN INTERSTITIAL POSITION OF THE
GALLIUM ARSENIDE LATTICE. Sándor Kunsági-Máté, Institute
for General and Physical Chemistry, Janus Pannonius University
Pécs, HUNGARY; Tamas Marek and Horst P. Strunk, Institute for
Microcharacterisation, Friedrich-Alexander-University
Erlangen-Nuremberg, GERMANY.

In low-temperature grown GaAs layers (LT-GaAs) the excess As
content depends on the substrate temperature and the As/Ga flux
ratio used during the deposition by molecular beam epitaxy (MBE).
The lower the temperature and the higher the As/Ga flux ratio, the
higher the As excess will be in the crystal. This fact relates to changes
in the interaction between As_2 molecules and Ga-terminated or
As-terminated GaAs(001) surfaces. To study this approaching process
energetically the path of an As_2 molecule towards the Ga-terminated
and also towards the As-terminated, planar, non-reconstructed
GaAs(001) surface was calculated. During our calculations the As_2
molecule is always oriented perpendicular to the (001) surface. We
represent the crystal by a $Ga_5As_2H_8$ (Ga-terminated surface) and by
a $Ga_2As_5H_8$ (As-terminated surface) cluster. The interaction energy
curve was determined by the total energy (Hartree-Fock, second order
Moller-Plesset correlation energy correction) of the system (cluster
plus molecule) for different heights of the As_2 molecule above the
surface. We did this calculations along the C_2 symmetry axis of the
system cluster plus molecule not only for positions above the surface
but also for positions in the surface plane and inside the crystal. In all
these positions the As_2 molecule lies on the C_2 symmetry axis and the
distance between its two As atoms is allowed to change. We show that
the system cluster plus molecule has a stable conformation only in
case of the As-terminated surface. In this situation the lower As atom
of the As_2 molecule lies in an interstitial position below the surface.
Finally, two more Ga atoms can reach the surface, making bonds with
the As atoms in the surface and with the upper As atom of the As_2
molecule. Thus, the two bonded Ga atoms confine the lower As atom
in an interstitial position. Therefore the process ends with an
energetically stable As-incorporated cluster.

2:45 PM N3.3
REAL-TIME MONITORING OF GaAs(001) MOLECULAR BEAM
EPITAXY USING SPECULAR ION CURRENT OSCILLATIONS
AND RECOVERIES. Kurt C. Ruthe, Paul M. DeLuca and Scott A.
Barnett, Northwestern University, Dept of Materials Science and
Engineering, Evanston, IL.

Low-energy glancing-angle Ar ions are used to examine the
homoepitaxial growth of GaAs(001) during molecular beam epitaxy.
In this technique, an ion beam impinges at glancing angles (1-5°)
relative to the sample surface, and the specular ion current is
measured. The specular ion current oscillated with monolayer growth
periods, and the specular ion current oscillations were simulated using
a rate equation model of two-dimensional epitaxy. The simulated
oscillations qualitatively agreed with the experimental observations by
assuming linear proportionality of ion scattering from surface defects.
The specular ion current recoveries allow a simple quantitative
interpretation based on scattering from step edges at various stages of
the growth oscillations. The scattered ion current increased gradually
upon closing the Ga shutter, and good fits to the recovery were
obtained by assuming a simple power-law island coarsening over a
range of monolayer coverages. For 0.1 ML/sec deposition on singular
GaAs(001) surfaces at 570°C, the fits indicate that the island density
increased with monolayer coverage from 6.4×10^{12} cm^{-2} at a coverage
of 0.18 ML up to a maximum of 1.1×10^{13} cm^{-2} at 0.35 ML and
subsequently decreased to 5.5×10^{12} cm^{-2} at a coverage of 0.62 ML.
Further, the measured average island area increased from
2.7 nm^2 to 11.4 nm^2 as the coverage increased from 0.18 ML to 0.62 ML.

3:30 PM N4.1
ATOMISTIC SIMULATION OF OXIDE FILM EVOLUTION
DURING MOCVD. Chaitanya Deo, Dept. of Materials Science &
Eng., University of Michigan, Ann Arbor, MI; David J. Srolovitz,
Princeton Materials Institute, Princeton University, Princeton, NJ.

Multicomponent oxide thin are becoming increasingly important for
microelectronic and electro-optic applications. While such films can
be produced using a wide range of deposition methods, MOCVD is
becoming the method of choice for producing high quality films at
reasonably high growth rates. In this work, we perform We present an
atomistic, 3-dimensional, kinetic Monte Carlo simulation results for
the MOCVD growth of such materials. We examine the growth of
these ordered structures on elemental, disordered, and ordered
substrates with low index surfaces. The as-grown films typically show
domains of ordered material separated by anti-phase boundaries.
Under some conditions, disordered films are observed. We examine
how growth rates and film structure (short-range order, vacancy
concentrations, domain sizes), morphology (including roughness) and
growth mode are affected by variations in reactor conditions; namely,
temperature, precursor partial pressures, and overall chamber
pressure). Finally, we use the simulations to construct a diagram of
growth mode versus reactor conditions.

3:45 PM N4.2
COMPUTER SIMULATION OF NUCLEATION AND GROWTH ON
PATTERNED SURFACES. A. Kuronen, L. Nurminen, K. Kaski,
Helsinki University of Technology Laboratory of Computational
Engineering, Espoo, FINLAND.

Many metal and semiconductor nanostructures have interesting
physical properties and they are expected to be of significant
technological importance in device fabrication. However, their
controlled manufacturing is a difficult task. One possibility is the
utilization of lattice mismatch between the substrate and thin film.
Many epitaxial systems exhibit a periodic arrangement of dislocations
that can be utilized as a patterned substrate for further film growth.
In other systems the lattice mismatch between the substrate and the
epilayer is manifested as a Moire structure. In this work we present
computer simulation studies on the effect of the patterned substrate
on the nucleation and growth of thin films. The structure and
energetics some model epitaxial systems are studied using the
molecular dynamics method. The nucleation and growth process is
simulated by the kinetic Monte Carlo method.

4:00 PM N4.3
REALIZATION OF DETAILED KINETIC MODELS FOR THE
GROWTH OF II-VI COMPOUNDS ADOPTING DFT
CALCULATIONS AND EXPERIMENTAL EVIDENCES.
Carlo Cavallotti, Valeria Bertani, Maurizio Masi, Sergio Carrá, Dept
Chimica Fisica Applicata, Politecnico di Milano, Milano, ITALY.

The possibility to link operating parameters of reactors adopted to
grow epitaxial layers with the physical and chemical properties of the
films is of great importance. Unfortunately, while the aim is clear, still
much work has to be done. A necessary step in this direction is the
comprehension of the elementary gas phase and surface chemistry
governing the film growth. Following this line of thought we adopted
quantum chemistry methods to study the reactivity of different
gaseous and surface species of interest for the deposition of II-VI
compounds. In particular we considered the CdTe and ZnS deposition
processes. All calculations were performed using density functional
theory methods such as the three parameters Becke-Lee-Yang-Parr
hybrid DFT method. The results of these studies enabled us to
improve our understanding of the elementary reactions that determine
the formation of the crystalline films. The link between atomic scale
calculations and reactor scale experimental data was obtained through
the realization of a detailed kinetic model. The kinetic constants of
the considered reactions were either found in the literature or
determined through transition state theory for the gas phase. For
surface reactions a first guess of the kinetic constant was done using
transition state theory (adopting energies calculated via quantum
chemistry methods) and then the parameters were slightly tuned (so
that they still retained a physical meaning) to give results in
agreement with experimental evidences. The predictive capability of
the kinetic models was tested simulating growth rates and gas phase
composition of experimental reactors differing from those adopted in
the fitting procedure.

4:15 PM N4.4
KINETIC LATTICE MONTE CARLO SIMULATION OF
POLYCRYSTALLINE THIN FILM GROWTH. Zhiyong Wang,
Arizona State University, Science and Engineering of Materials
Program, Tempe, AZ; James B. Adams, Arizona State University,
Department of Chemical, Bio and Materials Engineering, Tempe, AZ.

We present a three dimensional Kinetic Lattice Monte Carlo (KLMC)
simulation model which is capable of simulating polycrystalline thin
film growth including multiple grain orientations. The application of
this model to physical vapor deposition of metallic thin films is
discussed. Using this model, we study the microstructural evolution of
the metallic thin films as a function of deposition rate and substrate
temperature.

4:30 PM N4.5
EFFECT OF HYDROGEN COVERAGE ON SILICON THIN FILM
GROWTH: MOLECULAR DYNAMICS INVESTIGATION.
Shinya Muramatsu, Masatoshi Shimada and Masahiko Hirao, The
University of Tokyo, Department of Chemical System Engineering,
Tokyo, JAPAN.

Silicon thin film produced by CVD processes takes various structures
depending on reaction conditions. Hydrogen concentration of the
source gas affects the growth as well. In order to analyze the effect of
hydrogen coverage and substrate temperature on elementary surface
reactions, we performed molecular dynamics simulations, in which gas
phase radicals, H, SiH_2 and SiH_3, fell onto hydrogen-terminated
silicon surface. We prepared monohydride and dihydride Si(100)
surfaces and modified their hydrogen coverage of a certain area in the
range from 0.5 to 2 monolayers so as to simulate the reactions with
several kinds of surfaces which would appear in consequence of other
surface reactions. As a result of our simulation, hydrogen radical
caused adsorption and desorption reactions and altered hydrogen
coverage of the surface. While the reactions of SiH_2 and SiH_3 radicals
with monohydride or dihydride surface rarely occured, these radicals
reacted more frequently with the modified surfaces. These results
indicate that the change of hydrogen coverage caused by hydrogen
radical may induce subsequent surface reactions.

4:45 PM N4.6
REACTION LIMITED AGGREGATION IN SURFACTANT-
MEDIATED EPITAXY. Jing Wu, Bang-gui Liu, E.G. Wang, Institute
of Physics, Chinese Academy of Sciences, Beijing, CHINA; Zhenyu
Zhang, Oak Ridge National Lab, Oak Ridge, TN.

Reaction limited aggregation (RLA) theory is suggested to study the
surfactant effect on 2D island formation in homo- and hetero-epitaxy.
The epitaxial island is only stable after that adatoms exchange with
surfactant atoms by overcoming a large energy barrier, and
subsequent growth from such a seed is further limited by shielding
effect. Within this model, a fractal-to-compact island shape transition
can be induced by either decreasing the growth temperature or
increasing the deposition flux. This and other intriguing findings are
in excellent qualitative agreement wiht recent experiments.

8:30 AM *N5.1
NEW CONCEPTS IN MODELING EPITAXY USING THE
LEVEL-SET METHOD C. Ratsch, M.F. Gyure, HRL Laboratories,
Malibu, CA; R. Caflisch, S. Chen, M. Kang, B. Merriman, S. Osher,
M. Wheeler, UCLA, Los Angeles, CA; D.D. Vvedensky, Imperial
College, London, UNITED KINGDOM.

We develop an island dynamics model that employs the level-set
technique to describe epitaxial growth. The surface morphology is
described by defining the island boundaries as the set $\varphi = 0$ of the
so-called level-set function. The island boundaries then evolve with a
velocity that is obtained from solving the diffusion equation for the
spatially varying adatom concentration on the surface. Islands are
nucleated on the surface at a rate that is determined by the adatom
density. Scaled island size distributions in the submonolayer
aggregation regime are compared with those obtained from a kinetic
Monte Carlo (KMC) simulation for irreversible as well as reversible
aggregation. Excellent agreement is obtained. We identify spatial
fluctuations in the seeding of islands as an essential source of noise.
No other spatial or temporal fluctuations appear to be relevant. We
also show that the level-set method can naturally be extended to
multilayer growth, and give a quantitative comparison to data
obtained from KMC simulations.

9:00 AM N5.2

RATE EQUATIONS AND CAPTURE NUMBERS WITH IMPLICIT ISLAND CORRELATION. <u>Frederic Gibou</u>, UCLA, Dept of Mathematics, Los Angeles, CA; Christian Ratsch, UCLA, Dept of Mathematics and HRL, Los Angeles, CA; Susan Chen, UCLA, Dept of Mathematics, Los Angeles, CA; Mark Gyure, HRL, Malibu; Russel Caflisch, UCLA, Dept of Mathematics, Los Angeles, CA.

Mean field rate equations that form the basis of nucleation theory have been used for over 25 years to study epitaxial growth. One problem in using rate equations is that the functional form of the capture coefficients is not known. Several approximations for capture numbers are given in the literature; while some do correctly reproduce averaged quantities, none of these approaches have given the experimentally observed scaling of the island size distribution. We believe the reason is that spatial correlations between islands have been omitted and we propose a new way of computing numerically capture numbers including spatial correlation between islands: We use an island dynamics model that employs the level set technique, and find that the capture numbers are affinely dependent on the islands sizes. We numerically integrate the rate equations with these capture numbers, and compare our results with Kinetic Monte Carlo simulations. In particular, we focus on the island size distribution and island densities.

9:15 AM N5.3

A KINETIC MONTE CARLO MODEL OF SILICON-GERMANIUM CVD GROWTH. <u>M. Fearn</u>, J.H. Jefferson, M. Sayed and D.J. Robbins, Electronics Sector, D.E.R.A, Malvern, UNITED KINGDOM.

We report the development of a new atomistic scale Monte Carlo model of SiGe CVD thin-film growth from a mixed silane, germane and molecular hydrogen gas source. By employing a variable time step algorithm, simulations have been performed over a range of time scales, enabling direct comparison with experimental data. A multi-scale approach has been taken to provide physical data for the simulation model. Particle fluxes to the surface are derived from CFD calculations of the actual CVD reactor. The relevant surface reactions and their corresponding rates are derived directly using a combination of ab-initio atomistic modelling techniques and fitting to experimental data. Particular attention has been paid to surface diffusion which is important for a realistic simulation of SiGe growth. A simplified representation of diffusion has been incorporated efficiently into the MC scheme. The model is employed to study growth rates, alloy composition and surface concentrations of adsorbed species as a function of substrate temperature and gas source partial pressures. Surface hydrogen is known to desorb more readily off Ge sites than Si leading to an increase in surface sites available for adsorption. Consequently, in the growth of SiGe alloys, growth rates are sensitive to both surface composition and hydrogen coverage. To investigate this phenomenon further, ab-initio atomistic calculations are reported on the effect of surface hydrogen on the distribution of Ge atoms near the surface. This information is of direct benefit in enhancing the Monte Carlo model.

9:30 AM N5.4

EPITAXIAL GROWTH OF Au/Au (001) THIN FILM BY KINETIC MONTE CARLO SIMULATION. <u>Q.Y. Zhang</u>, State Key Laboratory for Materials Modification by Laser, Ion and Electron Beams, Dalian University of Technology, Dalian, CHINA; Z.Y. Pan, and J.Y. Tang Accelerator-based Atomic and Nuclear Physics Laboratory, Institute of Modern Physics, Fudan University, Shanghai, CHINA.

The behavior of Au/Au(100) thin film growth have been investigated by kinetic Monte Carlo simulation. The reentrant layer-by-layer growth during vapor phase epitaxial deposition of Au/Au(100) was observed in the temperature range of 450 K to 100 K. We revealed that the monomer diffusion plays a very important role in the vapor phase epitaxial growth. At low temperature, due to the limitation of monomers diffusion, adatom nucleation and island formation mainly depend on the increase of adatom by deposition randomly. With the increase of film growth temperature, the film growth mode depends on the competition between in-plane diffusion and inter-layer diffusion of monomers.

<div align="center">

SESSION N6: Si SUBSTRATES
Chair: Edward T. Yu
Wednesday Morning, December 1, 1999
Regis (M)

</div>

10:15 AM *N6.1

SELF-ORGANIZATION OF STEPS AND DOMAIN BOUNDARIES OF 7×7 RECONSTRUCTION ON Si(111). <u>H. Hibino</u>, Y. Homma, and T. Ogino, NTT Basic Research Laboratories, Kanagawa, JAPAN.

Recently, there has been a lot of interest in self-organized growth of materials. We have been investigating self-organization of steps and domain boundaries of the 7×7 reconstruction on Si(111) surfaces, because the steps and domain boundaries play special roles in epitaxial growth. Therefore, self-organized patterns of the steps and domain boundaries can be used as templates for the epitaxial growth. In this paper, we present three different aspects of the self-organization of steps and domain boundaries on Si(111) surfaces. First one is the formation of the triangular-tiled pattern of '1×1' and 7×7 domains during the phase transition. '1×1' and 7×7 domains have different surface stresses. The triangular-tiled pattern is stabilized through the stress relaxation. The second one is the step arrangement inside a hole which was fabricated by a standard lithographic technique. The step arrangement in the hole depends on the temperature. Below the '1×1'-to-7×7 phase transition, the hole has a three-fold symmetry consisting of step-bunched and non-bunched regions. This is because the step arrangement on the vicinal Si(111) surfaces depends on the direction of the steps. The last aspect is the formation of a pattern of steps and domain boundaries induced by Si growth. During the step-flow growth on Si(111), steps preferentially protrude along the domain boundaries on the lower terrace. The resulting changes in step shape induce a unique rearrangement of the domain boundaries, the number of which decreases during growth. However, when a periodic pattern is formed in the initial stages, it remains stable during growth.

10:45 AM N6.2

REAL-TIME OBSERVATION OF PT SILICIDE ISLAND MIGRATION BY PHOTOELECTRON EMISSION MICROSCOPY. <u>Woochul Yang</u>, H. Ade, R.J. Nemanich, North Carolina State Univ, Dept of Physics, Raleigh, NC.

The dynamics of the development of surface structures of Pt on Si(001) is investigated by photoelectron emission microscopy (PEEM). The photo electrons were excited with UV light from the free electron laser at Duke University or from a Hg discharge lamp. During in-situ annealing up to 1150°C, the morphology transition and island dynamics of Pt films of 1-20nm thickness are observed in real-time. For a 10nm Pt film, roughening and island formation of the Pt silicide films were clearly observed through the workfunction contrast PEEM. In particular, the formation of molten Pt silicide islands was observed below the melting point of PtSi. The PtSi film melting is related to the formation of Si-rich Pt silicide by Si diffusion into PtSi. In addition, the migration dynamics of the molten Pt silicide islands at 1100°C were monitored. The velocities of island migration were measured at different annealing temperatures. The temperature gradient of the Si substrate resulted in migration of molten islands from the edge to the center of the sample. The molten island dynamics is descirbed in terms of Si diffusion and/or surface tension.

11:00 AM N6.3

STUDIES OF THE FORMATION OF Ga AND Al NANO-STRUCTURES ON Si(112) SURFACES. <u>S.M. Prokes</u> and O.J. Glembocki, Naval Research Lab, Washington, DC.

We have studied the formation and growth of Ga and Al nanostructures on facet Si(112) surfaces (consisting of (111) terraces and (001) steps), investigated using LEED, Auger spectroscopy and Reflectance Difference Anisotropy (RDA). Ga or Al chains can form on this surface by a self-limiting process, which we can track from the rapid change from the (2x1) Si(112) reconstruction under sub-critical coverage, to chain formation leading to a 5x1 reconstruction followed by a 6x1 reconstruction. Using RDA, we have observed that depositions at or below 300C can lead to the formation of Ga or Al metallic wires on the Si(111) terraces, while at higher temperatures, the chains form only along the step edges and are not metallic, since each Ga is bonded to three silicon atoms at the step edge. Continued deposition to 9 overlayers (oL) at T below 250C leads to a large shift of the preferred polarization of the structure from along [-1-11] to along [1-10], while continued deposition in excess of 30 oL reverts back to polarization along [-1-11]. This result indicates that very anisotropic but patterned Al or Ga structures form at these low temperatures, retaining an unexpected large polarizability for coverage as large as 40 oL. This does not occur for depositions near room temperature or above 300C. Using atomic force microscopy (AFM), we have followed the changes in the RDA anisotropy in the 200-300C range, showing that as the RDA signal goes negative, metallic lines form on the Si(111) terraces. As the RDA signal passes through zero, the continued deposition leads to coverage of these lines by very small, isotropic Al (Ga) islands. With continued deposition, the RDA becomes positive and the AFM indicates the formation of elongated island structures along [-1-11], which form on top of the small, isotropic island structures.

11:15 AM N6.4

AB INITIO STUDY ON REACTION OF SILANE WITH Si(001).

Takahisa Ohno and Jun Nara, National Research Institute for Metals, Tsukuba, JAPAN.

Epitaxial growth of silicon on the Si(001) surface has attracted a great deal of attention due to its fundamental importance as a prototype system for understanding epitaxial growth and its technological application to numerous thin-film semiconductor technologies. Although the atomic processes involved in molecular beam epitaxy (MBE) have been intensively investigated, whereas little effort has been devoted to understanding the atomic processes of chemical precursors in chemical vapor deposition (CVD) growth. The decomposition of silane, SiH_4, on the Si(001) surface is one of the most important processes involved in CVD growth of epitaxial Si film, since silane is the most common precursor for Si. In this paper, we have investigated the interaction of silane with the Si(001)-(2x1) surface using first-principles total-energy calculations. It is found that silane molecules dissociatively adsorb on the Si(001) surface and that the SiHx fragments prefer to further decompose rather than to diffuse on the surface. The sequential decomposition of SiH_x species is suggested to lead to the formation of clean epitaxial Si dimers and paired H atoms on the substrate Si dimers. We will further discuss the dependence of the silane reaction on the local hydrogen coverage.

11:30 AM N6.5
MOLECULAR DYNAMICS SIMULATIONS OF SOLID PHASE EPITAXY OF Si: GROWTH MECHANISM AND DEFECT FORMATION. T. Motooka, K. Nisihira, Kyushu Univ, Dept of Materials Science and Engineering, Fukuoka, JAPAN; S. Munetoh, Sumitomo Metal Industries Ltd, Hyougo, JAPAN.

Crystal growth processes of Si during solid phase epitaxy (SPE) in the [001] direction have been investigated based on molecular dynamics (MD) simulations using the Tersoff potential. A tetragonal cell including an amorphous/crystalline (a/c) Si interface composed of approximately up to 6000 atoms was prepared as the starting system and was annealed at various temperatures. From the Arrhenius plot of the growth rates obtained by MD simulations, we have found that the activation energy of SPE at lower temperatures is in good agreement with the experimental value, approximately 2.7 eV while it becomes lower at higher temperatures. This can be attributed to the difference in the a/c interface structure and SPE mechanism. In the high temperature region, the a/c interface is predominantly composed of {111} facets and the rate-limiting step is a trapping process of Si at the kink sites associated with these facets. On the other hand, the a/c interface is essentially (001) in the low temperature region and the rate-limiting step is two-dimensional nucleation on the (001) a/c interface. Defect formation during SPE processes can be also observed and it was found that the defect formation was initiated by misorientations at the a/c interfaces resulting in various defect structures such as 5- and 7-member rings and (111) twins. Examples of atomic motions at the a/c interfaces during the SPE processes described above will be shown by a movie.

11:45 AM N6.6
DYNAMIC BEHAVIOR OF Si MAGIC CLUSTERS ON Si(111) SURFACES. Ing-Shouh Hwang, Mon-Shu Ho, and Tien T. Tsong, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan, R.O.C.

In a variable-temperature scanning tunneling microscope study of Si(111) surfaces, we find a special type of Si clusters which are not only stable with respect to surface diffusion, but are also the fundamental unit in mass transport phenomena, step fluctuations in detachment and attachment of Si atoms at step edges, and epitaxial growth. We characterize the structure of these clusters and derive path-specific hopping parameters using Arrhenius analysis. The magic clusters are also responsible for the decay of two-dimensional bilayer Si islands and Si craters at elevated temperatures. We also observe the decomposition of a small 5x5 island into several magic clusters. The concept of magic clusters may have important implication on the fundamental mechanism in epitaxial growth of many covalently bonded semiconductors.

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

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

In the last few years the scanning transmission electron microscope (STEM) has become capable of forming electron probes of atomic dimensions, as small as 0.13 nm in diameter. This has made possible a new approach to high-resolution electron microscopy, Z-contrast imaging. The Z-contrast image is an incoherent image, formed by mapping the intensity of high-angle scattered electrons as the probe is scanned across the specimen, and can be directly inverted to atomic structure. Because high angle scattering comes predominantly from the atomic nuclei, the scattering cross section depends on atomic number (Z) squared. The images therefore represent a direct map of the scattering power at atomic resolution. Z-contrast imaging is therefore an ideal technique to study compositional ordering at the atomic scale. In this presentation, examples are given of ordering in ferroelectric materials and III-V semiconductor alloys.
In ferroelectric materials, the atomic structure of ordered domains, both La-doped and undoped in $Pb(Mg_{1/3}Nb_{2/3})O_3$ is studied. The ordered domain structure in both cases is determined to be in agreement with the charge-balanced random-site model, and inconsistent with the space-charge model. It is shown that La doping in $Pb(Mg_{1/3}Nb_{2/3})O_3$ enhances not only the domain size but also the degree of ordering. In K-doped $PbZrO_3$, antiparallel cation displacements are observed but do not present any ordered structure. K is found to substitute for Pb uniformly in most ordered domains, while in some ordered domains, nonuniformly distributed K sites are also observed.
In III-V semiconductor alloys, spontaneous atomic ordering is common. It has profound effects on the electrical and optical properties of the materials. To understand the details of the ordered structures is important to understand their properties. Ordered structures in $GaAs_ySb_{1-y}$ and $Ga_yIn_{1-y}P$ are presented. In $GaAs_ySb_{1-y}$, a new ordered structure is observed, containing a periodic array of antiphase domains with Cu-Au ordering of the As and Sb atoms on the {110} and {100} planes. The antiphase domain boundaries are along the [110] direction and spaced by $2d_{110}$ of the zinc-blende structure. In $Ga_yIn_{1-y}P$, the ordered domains exhibit Cu-Pt ordering of As and P atoms. The ordered domains show two variants, [111] and [$\bar{1}\bar{1}1$] arranged periodically to form an orientational superlattice resulting in a discontinuity of the angular momentum. The structures of the antiphase domain boundaries, the orientational domain boundary and the interface between two ordered variants are discussed.

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

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

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

Artificial construction of atomically defined metal oxide layers is important in making electronic, magnetic, and optical devices. More recently, the fabrication of metal oxide self-organized quantum dots on metal oxide substrates has gained much attention because of their interesting physical properties such as ultraviolet laser emission. It is

experimentally well known that the formation of quantum dots is due to the large lattice mismatch beteen the substrate and thin film. This type of epitaxial growth is designated as higher-order epitaxy. The detailed understanding of the formation mechanism of self-organized quantum dots has been desired to control the size, shape, and crytallinity of the quantum dots. However, experimentally it is impossible to clarify the formation mechanism of the self-organized quantum dots on atomic scale. Hence, in the present study, we employed our crystal growth molecular dynamics simulator MOMODY [1-4] to simulate the formation process of various metal oxide quantum dots on sapphire(0001) surface. For example, when we continuously deposited MgO molecules on sapphire(0001) at 1000 K, the formation of MgO quantum dots was obserbed. The MgO quantum dots on sapphire(0001) has (111) orientaion and this formation process follows Stranski-Krastanov mode. Moreover, we suggested that the high flexibility of the coordination number of Al atoms on the topmost sapphire surface is a main reason for the higher order epitaxy and the formation of quantum dots. To the best of our knowledge, this is a first simulation study of the formation mechanism of self-organized quantum dots.

[1] M. Kubo, Y. Oumi R. Miura, A. Stirling, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and H. Koinuma, Phys. Rev. B 56 (1997) 13535.
[2] M. Kubo, Y. Oumi R. Miura, A. Stirling, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and H. Koinuma, J. Chem. Phys. 109 (1998) 8601.
[3] M. Kubo, Y. Oumi R. Miura, A. Stirling, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and H. Koinuma, J. Chem. Phys. 109 (1998) 9148.
[4] M. Kubo, Y. Oumi, H. Takaba, A. Chatterjee, and A. Miyamoto, J. Phys. Chem. B 103 (1999) 1876.

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

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

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

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

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

Large scale molecular dynamics simulations are performed to investigate the atomic-level surface stresses and migration processes on InAs/GaAs mesas. The simulations are based on an interatomic-potential scheme for mixed InAs/GaAs systems which depends on the local chemical composition. Multiresolution techniques are used to speed up the simulations. InAs/GaAs square mesas with {103}-type side walls and InAs/GaAs stripe mesas with {113}-type side walls are studied. Results will be presented for surface atomic stresses on the side walls with different monolayers of InAs, stress gradient on the side walls, and atomic-level distribution of hydrostatic pressure. Work supported by NSF, DOE, AFOSR, USC-LSU MURI, ARO, NASA, PRF, NSF USA-Japan International Grant, and LEQSF.

SESSION N8: POSTER SESSION
Wednesday Evening, December 1, 1999
8:00 P.M.
Exhibition Hall D (H)

N8.1
STATE SELECTED STUDIES OF DISSOCIATIVE CHEMISORPTION: PROBING THE MECHANISM OF GAS-SURFACE REACTIVITY. L.B.F. Juurlink, R.R. Smith, P.R. McCabe, C.L. DiCologero and A.L. Utz, Department of Chemistry, Tufts University, Medford, MA.

We will present recent experimental results that reveal how methane molecules in selected quantum states differ in their reactivity on single crystal nickel surfaces. We use infrared laser excitation to excite molecules in a molecular beam, and then quantify the reactivity of the state-selected molecules. These studies highlight how state-resolved studies of gas surface reactivity can reveal key features govern reactivity at the gas-surface interface.

N8.2
CALCULATION OF SURFACE ENERGY OF HCP CRYSTALS. Zinaida Matysina, Dnepropetrovsk State Univ, Dnepropetrovsk, UKRAINE; Dmitry V. Schur, Institute of Hydrogen and Solar Energy, Kiev, UKRAINE; Svetlana Yu. Zaginaichenko, Institute for Problems of Materials Science of NAS, Kiev, UKRAINE.

Knowing the surface energy in different lattice site planes of crystals can lead to prediction of the possible glide plane under crystal deformation if the mutual orientations of the directions for the external force and crystals basic vectors are known. Our work is aimed at the investigation of crystal surface energy of close-packed hexagonal structure for various crystallographic planes on the crystal-vacuum interface.
The fulfilled calculation is carried out in terms of molecular-kinetic representations using the broken bonds method. The interatomic interaction is taken into account in two coordinational spheres. The energy of different lattice sites planes of monocrystals is calculated and its angular relation defined. The calculations are carried out for relative surface energies of lattice site planes which make up the various angles with plane (0001) of Be, Hf, Ti, Zr, Mg, Co_α, Zn and Cd monocrystals which have the hexagonal close-packed lattice with axial ratio c/a $\neq$ 1,63. It is found that an increase in the c/a value lead to an increase in the surface energy.
The results of our calculations agree quantitatively with the known experimental data and the theoretical computations of other authors.

N8.3
INVESTIGATION OF ATOMIC STRUCTURE OF EPITAXIAL FILMS SURFACE. Svetlana Zaginaichenko, Inst for Problems of Materials Science of NAS, Kiev, UKRAINE; Zinaida Matysina, Dnepropetrovsk State Univ, Dnepropetrovsk, UKRAINE; Dmitry

Schur, Dmitry V. Schur, Inst of Hydrogen and Solar Energy, Kiev, UKRAINE.

The crystal surface structure of interface between the crystal and its surroundings which deal with the formation of texture is important in crystal growth theory. The surface of crystal may be flat lattice plane or it may have specific defects, and so be rough. For some external planes with sites, the crystal surface may have a complex stepline structure depending on the type of lattice and the indices of this plane. The energy of crystal depends on the structure of the latter and on the energies of the atomic interactions. Knowing the surface energy allows one to predict the type of free face arising in the process of monocrystal line growth, type of texture during polycrystal formation and the possible glide plane in case of deformation of a nondefective crystal, etc. Our work deals with the results of theoretical analysis of the crystal-melt interface. The crystal-melt boundary energy is calculated in the quasi-chemical approximation taking into account the correlation in the substitution of lattice sites by atoms and atomic interaction anisotropy.

The (100) face of the rhombohedral crystal lattice characteristic for the metals of the bismuth group is examined. The crystal is assumed to be in equilibrium with the melt. The existence of an interphase transition zone between the crystal and the melt is supposed. The calculated results for dependence of the change in free energy on the 'solid' concentration for cases with accounting for correlation and anisotropy and without for the latter are presented. The molecular roughness of the interface is determined. The effect of correlation and anisotropy on the crystal surface roughness is ascertained.

The comparison of our theoretical calculations with the known experimental data for bismuth and theoretical calculations of other authors are presented. The numerical analysis for bismuth permitted one to obtain some information about the atomic interaction in solid, liquid and different phases.

N8.4
ELECTRONIC STRUCTURE OF METALLIC SUPERLATTICES. SEMIEMPIRICAL CALCULATIONS. A.M. Mazzone, C.N.R.-Istituto LAMEL, Bologna, ITALY.

It is known that the usual growth modes of thin epitaxial films are scarcely descriptive of superlattices (SL) as these structures are very sensitive to the quality of the interfaces. Implicitly, this indicates that the usual thermodynamical parameters, used in epitaxis, are inadequate for SL design and therefore the synthesis of SL, with desired structural properties, depends ultimately upon the understanding of the fundamental properties of their electronic charge configuration.

However quantum mechanical calculations, which are expected to lead clarity into those problems, can not be applied to SL due to the size of these structures. The purpose of this study is to show that the problem may be circumvented by the use of a semiempirical method. Semiempirical methods play a major role in solid state physics and in quantum chemistry and it is generally thought that they lead to the characterization of large systems at the expense of details whose evaluation needs, by necessity, higher order calculations.

The method,used in our study, is at semiempirical level and hinges on the extended Debye-Hueckel approximation of the Hartree-Fock theory. The SL structure is represented as a large 'cluster' of a realistic thickness and of a limited transversal size. The cluster is formed by crystalline planes and its composition is of the type A/B with A,B=Ag,Cu,Pd and Fe. The calculations describe the binding energy of these structures and other fundamental parameters,such as charge overlapping and hybridization. The results suggest that a critical thickness exists. The evaluation of this parameter, though physically intuitive,is far from trivial as it arises from a balance between homopolar and heteropolar interactions.

The calculations are analyzed in the light of higher order spin polarized calculations on metallic surfaces whose details are also reported.

N8.5
EXTRACTING SURFACE FORCE-SEPARATION INFORMATION FROM HIGH-FREQUENCY SCANNING FORCE MICROSCOPY WITH MINIMAL HARDWARE CHANGES. Steven J. Eppell, Case Western Reserve University, Cleveland, OH; Fredy R. Zypman, University of Puerto Rico, Humacao, PR.

Advances in experimental scanning force microscopes (SFM) have prompted us to reassess the basic assumptions underlying current theoretical models used to convert SFM data into useful microscopic force-separation curves. These models are built upon the assumption that the cantilever-tip assembly behaves as a mechanical simple harmonic oscillator (SHO). A system properly described by these models can not naturally vibrate at more than one frequency. Multiple vibrational frequencies are excited during standard SFM operation [1]. Thus, it is not appropriate to obtain forces from measured displacements of an SFM cantilever using Hooke's Law

($F=-k.z$) unless it were known that the system vibrated at a single frequency. In order to solve this problem, previously, we proposed a method based on the analysis of the frequency spectrum as a function of separation [1].

In this new work we propose an improved, faster method that requires trivial modification of the current SFM hardware. The idea is to measure the reflection of a laser beam off a cantilever with a modulated light beam. From there the shape of the cantilever is retrieved and then, the force-separation curve. In this work we present the theory and the experimental setup. We also show the performance of our method to fall within few percent of the expected results, as opposed to the SHO that fail to reconstruct the Force-separation curves by as much as 100% beyond the snap-to-contact. [1] High Frequency Response of a Scanning Force Microscope Cantilever, Fredy R Zypman, Steven J Eppell, J Vac Sci Technol B16, 2099 (1998)

N8.6
MONITORING THE GROWING INTERFACE MORPHOLOGY OF A DEPOSIT THROUGH THE ROUGHNESS EXPONENT OF ATOMIC RESOLUTION STM OBSERVATIONS. H.-A. Durand, K. Sekine, K. Ito, K. Etoh, I. Kataoka; Japan Aviation Electronics Industry Ltd, Central Research Laboratory, Advanced Research Department, Tokyo, JAPAN.

We have been investigating the early moments of the formation of thin films on highly oriented pyrolytic graphite (HOPG) using an ultra high vacuum scanning tunneling microscope (STM) at atomic resolution. In a preliminary work, when carbon ions were deposited on HOPG, we first revealed a transition from island nucleation toward steady growth (deposit's on itself). We have studied the dynamic scaling of roughness of STM images as a function of deposit densities by electron beam evaporation on HOPG for nickel, molybdenum and a few other metals. A general model of evolution of the scaling exponent of roughness during the transition enables the monitoring of self-organized networks of nanoparticles deposited on a substrate. These investigations have specific importance for the control and production of materials enclosing metallic and semiconducting nanoparticles to be used in a new generation of magnetic and optoelectronic devices.

SESSION N9/I8: JOINT SESSION:
REAL-TIME IN-SITU STUDIES ON 3-D ISLANDING
Chair: Stephen J. Pennycook
Thursday Morning, December 2, 1999
Wellesley (M)

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

We have examined the growth and evolution of self-assembled Ge and GeSi islands on Si(001) using UHV transmission electron microscopy and low energy electron microscopy. The Ge/Si(001) system is of great interest because of the existence of two island shapes, shallow pyramids and more complex domes with steeper facets. In situ electron microscopy allows us to observe the development of these island shapes at video rate during growth by chemical vapour deposition, enabling us to distinguish between models for island formation.

After the nucleation of pyramidal islands, we observe a coarsening process which dramatically reduces the island density and increases the mean island volume. Surviving islands which reach a critical volume then change from the pyramid to the dome shape. We find that this shape change takes place slowly with the island passing through numerous asymmetric transition states having increasing numbers of higher angle facets. These asymmetric transition shapes can persist for several minutes, but they are temperature dependent and transform reversibly to the final dome shape during cooling. We can explain all our in situ results by using an anomalous coarsening model in which a process similar to Ostwald ripening occurs amongst an ensemble of islands whose equilibrium shape (pyramid, dome or transition shape) depends on volume. In this presentation we will show videos of island nucleation and growth and we will discuss this model. We will also describe how island development is modified by the strain fields of neighbouring islands and substrate dislocations. This is of interest since the use of substrate strain fields to pattern islands may allow us to develop uniform arrays of islands for new electronic applications.

9:00 AM *N9.2/I8.2

EPITAXIAL GROWTH OF GERMANIUM ON Si(001) - STUDIES BY HIGH TEMPERATURE STM DURING GROWTH. Bert Voigtlander and <u>Martin Kastner</u>, Institut für Grenzflachenforschung und Vakuumphysik, Forschungszentrum Julich, GERMANY.

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

9:30 AM *N9.3/I8.3

CHEMICAL ORDERING AT AND NEAR SURFACES: A UNIQUE INPUT OF GRAZING INCIDENCE X-RAY DIFFRACTION <u>Michele Sauvage-Simkin</u>, LURE, Orsay, FRANCE and Laboratoire de Minèralogie-Cristallographie, Paris, FRANCE.

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

10:15 AM *N9.4/I8.4

IN-SITU MEASUREMENTS OF STRESS RELAXATION DURING STRAINED LAYER HETEROEPITAXY. <u>E. Chason</u>, J. Yin, K. Tetz, R. Beresford, E. Chen, D. Paine, L.B. Freund, Brown University, Providence, RI; J.A. Floro, Sandia National Laboratories, Albuquerque, NM.

Stress plays a critical role in determing the evolution and the properties of heteroepitaxial layers. Stress-induced morphological changes such as island formation can prevent the formation of sharp interfaces. Dislocations that form to relieve the stress can severely degrade the electronic properties of the layer. Although there has been much work done on the energetics of stress relaxation, the kinetics of stress relaxation have not been studied as intensively because of the difficulty of obtaining real-time data. In this talk, we will discuss measurements of dislocation-mediated stress relaxation in layers of InGaAs grown on GaAs (001) performed during growth.

These results were obtained using a novel wafer-curvature based technique optimized for in situ studies. At high temperature or stress, the layers relax continuously above the critical thickness, while for low temperatures or stress, the films grow pseudomorphically over a much larger region of metastability before relaxing rapidly. In addition, we find that relaxation occurs without additional growth above a certain thickness. By comparing measurements made with and without growth interrupts, the relaxation at constant thickness can be separated from the relaxation during growth. The degree of relaxation induced by growth interrupts at constant temperature and at elevated temperature is compared with the stress evolution during continuous growth. Results are interpreted in terms of models of dislocation-mediated relaxation. Portions of this work were performed at Sandia National Laboratory and supported by the United States Department of Energy under contract DE-AC04-94AL8500.

10:45 AM *N9.5/I8.5

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

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

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

DAVID TURNBULL AWARD LECTURE

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

Surface reaction pathways and kinetics of $Si_{1-x}Ge_x$ growth on Si(001) by both gas-source MBE (GS-MBE) and atomic-layer epitaxy (ALE) from Si_2H_6/Ge_2H_6 mixtures have been investigated using a combination of $in-situ$ RHEED, EELS, STM, STS, TPD, and AES together with post-deposition TEM, HR-XRD, XTEM, and electronic transport measurements. Film growth data are well described by models containing separate reaction steps for dissociative chemisorption, surface reactions, and hydrogen desorption. For UV-photostimulated ALE, hydrogen termination provides internally self-limiting kinetics and allows epitaxial growth at room temperature and below.
The results of isotopically-tagged D_2 temperature-programmed desorption (TPD) experiments were used to model temperature-dependent H-mediated effects of high B coverages on the growth kinetics of B ultra-high doped $Si_{1-x}Ge_x(001)$, up to 1.5×10^{22} cm^{-3} (30 at%), through changes in B-induced surface reconstruction and back-bond charge transfer, and to determine Ge segregation kinetics as a function of x and steady-state H coverage during GS-MBE. Excess incorporated B does not precipitate out of solution as commonly supposed. Rather, our recent NEXAFS and HR-XRD results, carried out at the Synchrotron Radiation Center in Stoughton, show it is incorporated as sp^2 bonded dimers with trigonal symmetry on substitutional Si sites. The dimers are bond-saturated and thus electrically neutral. Further, they have very low charge scattering cross-sections.

1:30 PM *N10.1
MODELING OF STRUCTURAL AND ELASTIC PROPERTIES OF
$In_xGa_{1-x}N$ ALLOYS. Frank Grosse, Jörg Neugebauer,
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin,
GERMANY.

We have investigated the structural and elastic properties of ordered
and random $\{In_xGa_{1-x}N\}$ alloys by combining density-functional
theory (DFT) calculations and valence force field models. Employing
first-principles calculations a large number of ordered $\{In_xGa_{1-x}N\}$
alloys with different compositions and geometries have been studied.
Based on these results we have extended the valence force field (VFF)
model [1,2] by fully taking the ion-ion interaction into account (ZVFF
model). The new method has several advantages compared to the
traditional VFF model: it correctly describes the energy differences
between the stable wurtzite and the metastable zincblende phase and
the existence of inequivalent bonds in the wurtzite phase resulting e.g.
in non-ideal c/a ratios. Applying the ZVFF model to large supercells
the wurtzite phase is found for all In concentrations stable against the
zincblende phase, in contradiction to previous theoretical results [3].
Furthermore, we identify structures with low formation enthalpies as
candidates for chemical ordering in $\{In_xGa_{1-x}N\}$ alloys. They differ
from common [0001] superlattices with full layers of In and Ga,
respectively. Finally we have studied the change of the elastic
constants with In concentration and deduced the elastic bowing
coefficients. Based on our results it is possible to determine the
averaged concentration in epitaxial layers by simultaneous
measurements of the a and c lattice constant. [1] P.N. Keating, Phys.
Rev. **145**, 637 (1966). [2] R.M. Martin, Phys. Rev. B **1**, 4005 (1970).
[3] M. van Schilfgaarde, A. Sher, and A.-B. Chen, J. Crystal Growth
178, 8 (1997).

2:00 PM N10.2
EMBEDDED ATOM MODEL OF THE RECONSTRUCTION OF
Au(100) IN AN ELECTROCHEMICAL ENVIRONMENT.
Michael I. Haftel, Naval Research Laboratory, Washington DC and
University of Maryland, College Park, MD; Mervine Rosen, Naval
Research Laboratory, Washington, DC.

We apply a recently-developed model of the metal-electrolyte
interface, based on the surface-embedded-atom-model (SEAM), to the
quasihexagonal reconstruction of Au(100). We calculate the Gibbs
free surface energy of the 1x1 and reconstructed phases as functions of
the electrochemical potential relative to the potential of zero charge
(PZC). The SEAM predicts a lifting of the reconstruction about 0.2 V
positive of the PZC of the 1X1 phase compared to the experimental
value [1] of 0.50 V and the density-functional result[2] of no lifting of
the reconstruction at all. We then describe an alternate approach
based on a thermodynamic formulation, measured capacities, and
theoretical calculations of the surface energy for zero charge. This
approach indicates a transition potential between +0.2 and +1.0 V
(PZC) thus suggesting that charge effects, and not just anion
absorption effects, play a role in lifting the reconstruction. 1. D.M.
Kolb, Prog. Surf. Sci. 51, 109 (1996). 2. K.P. Bohnen and D.M. Kolb,
Surf. Sci. 407, L629 (1998).

2:15 PM N10.3
QUANTUM CHEMICAL CALCULATIONS ON THE
INTERACTION OF NF_3 WITH Si SUBSTRATE. Akira Endou,
Aruba Yamada, Seiichi Takami, Momoji Kubo, Akira Miyamoto,
Graduate School of Eng., Tohoku Univ., Sendai, JAPAN; Masahiro
Kitajima, National Research Institute for Metals, Tsukuba, JAPAN;
Thomas W. Little, Fumio S. Ohuchi, Dept. of Materials Science and
Eng., Univ. of Washington, Seatle, WA.

A significant amount of work has been reported on etching rate and
reaction mechanism in NF_3 plasma etching of Si and SiO_2. Little et
al. studied the interaction of NF_3 with Si surface by x-ray
photoelectron spectroscopy and suggested the presence of both Si-F
and Si-N bonding for NF_3 ion beam interaction and probably F-N-Si
moieties [1]. However, the exact nature of the bonding has not been
clarified and theoretical studies concerned with this system have not
appeared yet. In this study, the possible cases of NF_3 interaction with
Si substrate have been investigated by density functional quantum
chemical calculations. We used the $Si_{10}H_{16}$ cluster model as the
representatives of H-Si(100)-1x1 and H-Si(111) 1x1 surfaces. Our
results show that fluorine atom in T_d site is not stable at the ground
state. Adsorbed F atom on Si surface as well as F at the interstitial
sites indicated large negative charges and the Si-F bonds formed on
silicon surface resemble those of SiF_4 molecule. In the case of the
NF_3/Si system, the negative charges on the F atoms bound to Si=N
or Si-N< were found to be less and this is in full accordance with the

reported experimental results. [1] T.W. Little and F.S. Ohuchi: Mat.
Res. Soc. Symp. Proc., **438**(1997) 251.

2:30 PM N10.4
EPITAXIAL GROWTH MODE TRANSITIONS INDUCED BY A
SCHWOEBEL EFFECT. Vladimir Trofimov, Vladimir Mokerov, Inst
of Radioengr & Elec of RAS, Moscow, RUSSIA.

Recently we have developed [1] a simple self-consistent model for
homoepitaxial layer growth kinetics that takes into account the
existence of a Schwoebel barrier at an island edge by using a concept
of a feeding zone, proposed our earlier [2]. In this paper, we extend
the model to the case of heteroepitaxy (without lattice mismatch) by
introducing different adatom surface diffusion coefficients in the first
layer (heterodiffusion) and in the all next layers (self-diffusion).Model
consists of an infinite set of coupled non-linear rate equations for
adatom and 2D island surface densities and coverage in successive
growing layers.These equations in combination with an integral
condition for a new layer nucleation fully describe epitaxial growth
kinetics on a singular surface at predetermined six model parameters,
characterizing adatom hetero/self diffusion rate, critical nucleus size
and stability, Schwoebel effect, and coalescence behaviour,
respectively. By numerical integration of these equations in a wide
range of model parameters growth mode transitions are studied in
detail and phase diagrams of the growth modes in various parameter
spaces are constructed. Comparison with available experimental data
are given as well.
1. V. Trofimov et al. MRS 1998 Fall Meeting Abstracts, C2.3; E-MRS
1999 Spring Meeting Abstracts, C-I/P29. 2. V.I. Trofimov, V.A.
Osadchenko, Growth and Morphology of Thin Films (in Russian),
Moscow, Energoatomizdat, 1993, 272pp.

3:00 PM *N11.1
NANOSCALE ELECTRON-BEAM PROCESSES AND ITS
APPLICATION TO NANODEVICES. Masanori Komuro,
Electrotechnical Laboratory, Ibaraki, JAPAN.

Finely focused electron-beam(EB) processes are very attractive and
powerful method for producing nanometer-scale structures for
advanced electron devices such as single electron transistor(SET).
Here in this talk, nanometer-scale structure formations using
inorganic resist and EB-induced metal deposition are described,
aiming at high temperature operation of SET based on
metal/insulator/metal (MIM) tunnel junctions. In the inorganic resist
process, thermally oxidized silicon layer is used as a positive resist
where electron irradiated area is readily solved in buffered HF
solution. Although the sensitivity of the resist is about a few C/cm^2
which is lower than conventional resists, it is possible to delineate fine
line and space pattern with 15 nm pitch and 5 nm width. This
technique is extended to make miniature MIM junctions using
SiO_2/Si bilayer resist and the following multi-angle deposition
method. Metal layer is directly deposited on SiO_2 substrates in WF_6
gas ambient simultaneously with EB irradiation. The resistivity of the
deposited film is about $6x10^{-4}$ Ohm-cm depending on hydro-carbon
contamination of the substrate itself. We can make the deposited lines
with line-width of about 10 nm using 3 nm diameter of the incident
EB. From current-voltage characteristics for single tunnel junctions
with various tunnel resistances, the barrier height is estimated to be
about 0.2 eV. This result indicates clearly the junction properties can
be controlled at least with the accuracy of minimum deflection
increment of the EB system used here. It is successfully observed that
the SET produced by EB-induced deposition exhibits Coulomb
oscillation at temperature of 230 K.

3:30 PM N11.2
STEP BUNCHING DURING SiGe GROWTH ON VICINAL Si(111)
SURFACES. H. Hibino and T. Ogino, NTT Basic Research
Laboratories, Kanagawa, JAPAN.

Step bunching on strained layers has been observed, and it was shown
that the elastic attractive interaction between steps on the strained
layer surface leads to a bunching instability. In this paper, we describe
the influence of growth conditions on step bunching during SiGe
growth on vicinal Si(111) surfaces, and discuss the important factors
controlling the step bunching. We first investigated the influence of
the Ge concentration, θ, on step bunching during SiGe growth at
550°C. 10-nm-thick SiGe layers with θ lower than 50% were grown on
vicinal Si(111) surfaces misoriented by 2°. The number of the
bunched steps, N, increases as θ increases. However, these results do

not agree very well with the dependence of N on θ expected from the theory of the stress-induced step bunching. Additionally, we measured the dependence of N on the SiGe thickness, and find that N attains a saturated value after the growth of 10-nm-thick layers. The saturation is also confirmed by the observation of two-dimensional islands on the terraces. These results suggest that N is mainly decided by the diffusion of adatoms, and that the diffusion length depends on θ. The diffusion length increases with the temperature, and therefore, N increases dramatically with increase in temperature. We also discuss another effect of stress in stress-induced step bunching. During Si growth on vicinal Si(111) surfaces on which steps have already been bunched, the lowest step in the step bunch advances faster than the rest of the step bunch. This crossing step limits the subsequent step bunching. In contrast, during SiGe growth, two-dimensional island formation limits the step bunching. We believe that, during SiGe growth, it is difficult for atoms to attach to the lowest step in the step bunch, because the lowest step is more strained than the rest of the steps

3:45 PM <u>N11.3</u>
EPITAXIAL GROWTH AND IN-SITU CHARACTERISATION OF Mo(111) ON SAPPHIRE(0001). <u>P.A. Ryan</u>, F. Tsui, Dept of Physics and Astronomy, University of North Carolina, Chapel Hill, NC.

Mo (111) films have been investigated using real-time Reflection High Energy Electron Diffraction (RHEED), in-situ non-contact AFM and STM. The films were deposited on Sapphire (0001) substrates by MBE, at substrate temperatures between 200 and 1000°C and rates from 0.01 to 3Ås. The RHEED images indicate an initial roughening of the surface as the Mo is deposited. However, at a thickness of 15Å the RHEED specular reflectivity exhibits a peak, indicating a smoothening of the Mo surface. This smooth surface is confirmed by in-situ AFM images. The diffusion length of Mo atoms on this smooth surface appears to increase substantially. Films of this thickness have been investigated using in-situ STM and conductance measurements. These indicate an insulator to metallic phase transition, in agreement with the increased diffusion length of the Mo atoms on the surface. The thickness at which the Mo becomes smooth is unaffected by the deposition temperatures or rate. However, the intensity of the specularly reflected RHEED beam, which is an indication of the smoothness of the layer, depends on both the rate and temperature. For each temperature, the optimal rate for the smoothest layer has been determined. As the deposition temperature was increased the optimal rate increased, indicating a kinetic process. Subsequent deposition onto the smooth surface shows a continuous roughening of the film.

4:00 PM <u>N11.4</u>
SECOND DERIVATIVE BALLISTIC ELECTRON EMISSION SPECTROSCOPY IN Au/(AlGa)As. <u>Michael Kozhevnikov</u>, Venky Narayanamurti, Harvard Univ, Gordon McKay Lab, Cambridge, MA; Darryl L. Smith, Los Alamos National Lab, Los Alamos, NM; Yi-Jen Chiu, Univ of California at Santa Barbara, Electrical and Computer Engineering Dept, Santa Barbara, CA.

Ballistic Electron Emission Microscopy (BEEM), a three-terminal modification of Scanning Tunneling Microscopy (STM), is a powerful low-energy tool for nondestructive local characterization of semiconductor heterostructures. The energy and angular distribution of hot electrons (or holes) can be controlled independently on the semiconductor structure by varying the tip potential. Thus BEEM provides, in complement to the surface morphology, a new form of low-energy electron/hole microscopy and spectroscopy with high spatial and energy resolution. Recent research in our laboratory has established BEEM electron (and hole) transport in buried semiconductor structures on the nm scale in a low energy regime of $\sim$1 eV with energy resolution of $\sim$10 meV. The focus of our current study is on the analysis of the second derivative (SD) BEEM spectra of Au/(AlGa)As heterostructures to estimate quantitatively the effect of the carrier scattering in the metal, at the metal-semiconductor (m-s) interface and in the semiconductor on the multivalley carrier transport. The SD-BEEM spectra, representing the heterostructure transmission coefficient, show explicit partitioning of the contribution of different transport channels (Γ, L and X conduction valleys). Our analysis of SD-BEEM spectra in the frame of the developed theoretical model indicates that about 90% of the BEEM electrons are scattered at the nonepitaxial Au/GaAs interface. We also show that initial electron distribution among the conduction bands of the semiconductor, specified by the m-s interface scattering, is modified by the further hot-electron transport inside the semiconductor. As the heterostructure, characterized by several transport channels, is buried deeper, the contribution of these conduction channels decreases gradually, starting from the transport channel with the shortest electron mean free path length in semiconductor.

4:15 PM <u>N11.5</u>
THE GROWTH OF METALS ON TiO_2(110): EVIDENCE FOR SELF-LIMITED COPPER ISLAND SIZES. <u>D.A. Chen</u>, University of South Carolina, Department of Chemistry and Biochemistry, Columbia, SC; S.M. Seutter, M.C. Bartelt, R.Q. Hwang and K.F. McCarty, Sandia National Laboratories, Livermore, CA.

Metal-oxide interfaces play an important role in a variety of materials and chemical applications. In order to develop a fundamental understanding of these interfaces, we have studied the nucleation and growth of Cu islands on rutile TiO_2(110)-(1x1) in ultrahigh vacuum using scanning tunneling microscopy. The formation of 3D islands reflects the relatively high mobility of Cu atoms on TiO_2 at room temperature and the weak interactions between Cu and TiO_2. At low coverages ($\leq$0.5 ML), Cu islands exhibit self-limiting growth since the average island size remains essentially constant with increasing coverage while the island density increases. At the higher coverages ($>$0.5 ML), the average island size scales with coverage, but this increase in island size is primarily due to an increase in height, not diameter. Although larger islands can be formed by annealing, the average size of the islands is independent of coverage for any given annealing temperature. Two general scenarios are proposed to explain this self-limiting island growth: either the rate at which adatoms attach to existing islands drops as the island size increases; or the rate at which adatoms reach existing islands drops as Cu coverage increases. Simulations for lattice gas models show that both scenarios can account for the observed increase in island density with increasing coverage and the narrow size distribution. We will also compare the growth of Cu islands with our studies of less reactive (Ag) and more reactive (Cr) metals on TiO_2(110). This work was performed under the U.S. Department of Energy contract DE-AC04-94AL85000 and supported in part by the USDOE-OBES-Division of Materials Sciences.

4:30 PM <u>N11.6</u>
IMAGING BURIED INTERFACIAL LATTICES WITH QUANTIZED ELECTRONS. <u>Dongmin Chen</u> and Igor Altfeder, The Rowland Institute for Science, Cambridge, MA.

Electrons under spatial confinement in a nanoscale system exhibit fascinating wave properties. Our recent experiment using a low temperature STM has shown that electron interference fringes can form spontaneously on the surface of a thin epitaxial metal film grown on a stepped Si(111) substrate. Imaging these interference fringes together with the STS measurement of the respective quantization energy spectra provides us with a nondestructive technique for a complete three dimensional characterization of both the buried interface morphology and the burial layer of a heteroepitaxial system. More surprisingly, the experiment reveals that the well known Si(111)7x7 superlattice buried under as much as 100 angstroms of Lead film can be directly imaged on the metal surface by the STM. Theoretical analysis shows that such an unexpected high ballistic resolving power is facilitated by a non-diffractive scattering of the conduction electrons at the interfacial defects as a result of a large anisotropic motion of the electrons in a 2D nano structure. Refernces: 1. I.B. altfeder, D.M. Chen and K.A. Matveev, Phys. Rev. Lett. 80, 4895(1998); 2. I.B. Altfeder, K.A. Matveev and D.M. Chen Phys. Rev. Lett. 78, 2815 (1997).

4:45 PM <u>N11.7</u>
A SCALING MODEL TO UNDERSTAND THE NANOSCALE TRANSITION FROM HETEROGENOUS TO HOMOGENOUS GROWTH OF METALS ON HOPG. <u>H.-A. Durand</u>, K. Sekine, K. Ito, K. Etoh, I. Kataoka, Japan Aviation Electronics Industry Ltd, Central Research Laboratory, Advanced Research Department, Tokyo, JAPAN.

We have been investigating the early moments of the formation of thin films on highly oriented pyrolytic graphite (HOPG) using an ultra high vacuum scanning tunneling microscope (STM) at atomic resolution. In a preliminary work, when carbon ions were deposited on HOPG, we first revealed a transition from island nucleation toward steady growth (deposit's on itself). We have studied the dynamic scaling of roughness of STM images as a function of deposit densities by electron beam evaporation on HOPG for nickel, molybdenum and a few other metals. A general model of evolution of the scaling exponent of roughness during the transition enables the monitoring of self-organized networks of nanoparticles deposited on a substrate. These investigations have specific importance for the control and production of materials enclosing metallic and semiconducting nanoparticles to be used in a new generation of magnetic and optoelectronic devices.