FACETS OF HETEROEPITAXY: THEORY, EXPERIMENT, AND COMPUTATION

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1 Introduction

The word epitaxy comes from the Greek words *taxis* meaning in an ordered manner and *epi* meaning above. For our purposes epitaxial growth is a process in which thin films are grown in a vacuum by deposition onto a crytalline substrate. The deposition is, relatively speaking, slow and the resulting film is also crystalline (well ordered). There are basically two types of epitaxial growth, namely homoepitaxial growth and heteroepitaxial growth. In the former, the deposited material is the same as that of the substrate. In heteroepitaxial growth, atoms of different species are deposited on to a substrate of different type (which also may be composed of a various atomistic species i.e. an alloy). One prototypical system is Germanium deposited on Silicon.

One significant difference between homoepitaxial and heteroepitaxial growth are elastic effects. These arise because the natural bond length of the deposited species often are different from the substrate. The effects on film growth can be dramatic since the system can lower its elastic energy by forming mounds (sometimes called three dimensional islands) while at the same time remaining a coherent solid (i.e. no dislocations form). However, the mound formation will increase the surface energy. Therefore the morphology of the growing film is determined not only by kinetic effects but also by the thermodynamic competition between surface energy and elastic energy (which is a bulk effect). In many systems it turns out that the system can lower its total energy forming these mounds. Therefore, we see that the mounds are self-assembled. Not only are such systems intrinsically interesting but they also are important from a technological perspective. This is because the mound size can be on the order of tens of nanometers. Mounds this small are often called quantum dots. Such quantum dots have interesting optical and electronic properties. For example solid state lasers have been made using such materials.

An ambitious goal would to be to predict the film composition and morphology under a wide variety conditions. A more modest goal would be to a least understand the experiments and suggest new experimental parameters or materials to consider. From a theoretical point of view, either of these goals is an enormous challenge. One fundamental difficult is the vast range of time scales and length scales that must be properly treated in order to have faithful models. For example, if one would like to simulate an epitaxial system with molecular dynamics then the time and length scales are on the order of 10^{-12} sec and 10^{-4} microns (atomistic scale). However, we need to understand the system on the scale of seconds and microns (macroscale). To complicate matters there are processes that occur on this small scale that can have direct consequences on the macroscale. It should be pointed out that much of the current understanding is still driven by experimental results. For example, the notion that one could have self-assembled islands driven by misfit strain was first

seen experimentally and was very surprising from a theoretical perspective. The wisdom at the time was that dislocations would provide stain relief.

There are many issues involved in improving our understanding of epitaxial growth from a mathematical point of view. However one can not make progress without working closely with experimentalists. Probably the single most important issue is modeling. There are many different types of models ranging from atomistic which are discrete in nature to coarse-grained models which are typically phrased in terms of partial differential equations. One advantage of atomistic models is that the need to model is considerably reduced. For example, if one is using molecular dynamics all that is required is a model of the intermolecular potential. As one proceeds to coarse-grain the problem more and more information is needed. The advantage is that one achieves not only greater understanding but also a more efficient description. The problem of coarse-graining atomistic problems is incredibly difficult but is central to the issue of modeling and simulation of epitaxial growth. However little progress can be obtained without working closely with experimentalists. The aim of this workshop was to bring together a diverse group: people who focus on computational aspects, experimentalists, and those who develop models.

2 Meeting Content

2.1 Overview Talks

The workshop began with two overview talks.

Overview Talk 1. The first was by Jerry Tersoff who spoke on the basic issues involved in modeling heteroepitaxial growth using continuum models. He outlined the important interplay between elastic energy, surface energy, anisotropic effects, intermixing, and surface segregation. He described situations where the form of the anisotropic surface energy would permit barrierless formation of faceted islands for a rippled surface.

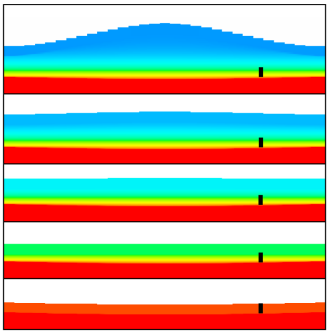

FIG. 1 (color online). Evolution of structure and composition during heteroepitaxy, for nominal $Si_{0.60}Ge_{0.40}$ on Si(001), at deposition rate of 10^4 (arbitrary units). The onset of nonplanar morphology is more abrupt at lower growth rates. Colors indicate composition, from pure Si substrate (bottom) to $Si_{0.62}Ge_{0.38}$ (top). The bottom panel is the initial surface (slightly nonplanar), and subsequent panels are at equal time intervals. The figure shows one unit cell of periodic system; the lateral size is $640w_s$. Surface-layer thickness w_s is indicated by a black rectangle in bottom panel; the vertical scale is greatly expanded to show the small perturbation. The rectangle is repeated in the same position in subsequent panels for reference. Surface steps are a graphical artifact.

Figure 1: This figure is from [1] and was discussed in Jerry Tersoff's overview talk.

His talk also discussed his recent work with Y. Tu which showed that segregation could play an important role in the morphology of the growing film. [1, 2, 3] An interesting feature of this work is that the model suggests that wetting layer in Stranski-Krastinov (SK) growth should really be thought of as a transition thickness where the growth rate increases dramatically. In this way, they are claiming that SK growth is really a kinetic effect. This view departs from the conventional wisdom, and sparked a spirited discussion of experimental and theoretical results that both refute and support this hypothesis.

Overview Talk 2. The second overview talk was by Tom Tiedje who presented both experimental results and a model for the epitaxial growth of Gallium Arsenide. [4]. However, the model developed is relevant to any homoepitaxial system. It was based on a combination of physical intuition and experimental results. Experimental results showed that in the growth regimes considered the film was better modeled by an Edwards-Wilkinson model rather than surface diffusion (Mullins). A nonlinear term, based on physical principles, due Villain was added.

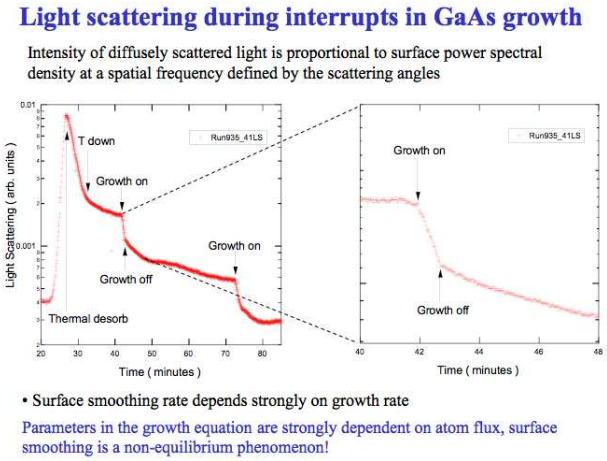

Figure 2: Light scattering data for the growth of GaAs homoepitaxial films. In these experiments, the surface continues to evolve even after the growth flux is removed, and has important implications for the development of appropriate models (from Tom Tiedje's talk).

In addition, effects of a step-edge barrier were included by incorporating a current. An interesting feature of the model present was the inclusion of effects of nucleation which allows one to study both island growth and step flow. The model was also in good agreement with kinetic Monte Carlo.

2.2 Regular Talks

The remainder of this review provides a summary of the talks in the order they were given.

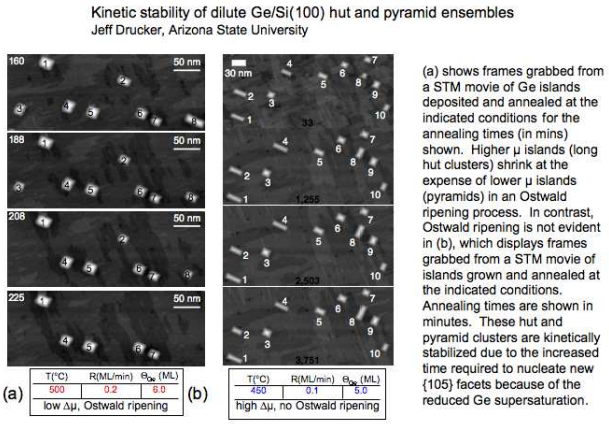

Figure 3: A slide from Jeff Druckers talk showing frames of a movie made by a scanning tunneling microscope (STM) that demonstrates the evolution of islands on the surface.

Jeff Drucker. This talk began by presenting experimental results of the Ostwald ripening of Ge/Si huts and pyramids. [5] These results were based on in situ STM. It was observed that the huts were less stable than

the pyramids and the presence of a large dislocated island would alter the ripening of the small islands. Many features of the experiment were modeled by a mean field nucleation theory.

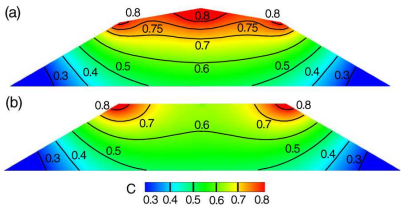

FIG. 4 (color online). Equilibrium composition profiles in axisymmetric quantum dots with (a) "dome" shape, the angles of the sidewalls being 30° and 15°, and (b) a truncated-cone shape with a sidewall angle of 30°. While the composition profiles are similar near the base, larger strain relaxation in the regions near the corners results in a greater segregation in the apex of the dome-shaped quantum dot. The composition profiles are obtained for $F_0 = -0.2$ and $\bar{c} = 0.5$.

Figure 4: This figure is from [6] and was discussed in Vivek Shenoy's talk.

Vivek Shenoy. Work was presented in which composition maps of quantum dots were numerically computed using a continuum model. The model was based on minimizing the total free energy using a finite element method. The results suggested that shallow pyramids do not have extreme composition profiles whereas steeper islands would have high concentrations of Germanium near the top. There was some discussion on the relationship of these energy minimizing solutions as compared to experimental results especially in the of kinetic effects.

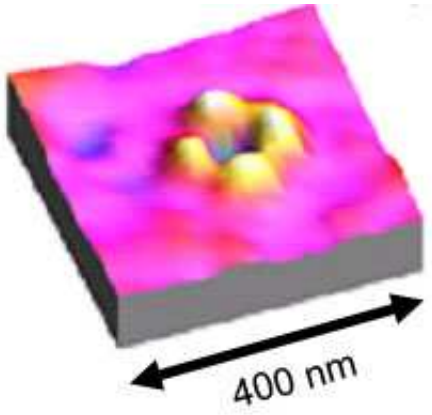

Figure 5: An AFM image showing a new class of nanostructure discovered by Gray, Hull, and coworkers, the quantum fortress. It consists of a pit surrounded by discrete islands.

Robert Hull. In his talk the speaker presented some novel self assembled nanostructures comprised of pits surrounded by multiple quantum dots, which occur in a very narrow regime of experimental conditions. One feature of these conditions is that the adatoms have limited mobility. It is hoped that such structures will have applications in quantum cellular automata, spin exchange and coherent spin exchange switches. This was joint work with Jennifer Gray (a workshop participant). Relevent material can be foound in Ref. [7].

Ernesto Placidi. Features quantum dot transitions in InAs/GaAs were discussed in this talk. [8] It was experimentally determined that volume of the quantum dots exceeds that of the material deposited from which is was speculated that the extra material must come from intermixing with the substrate, most likely from adatom detachment from step edges from the surface steps. **Jim Evans.** Evans discussed homoepitaxy

of silver on silver, which gives rise to very interesting film morphology due its large step edge barriers (see Figure 2.2). He showed how the strength of the step edge barrier can be inferred from the island shape [9]. He

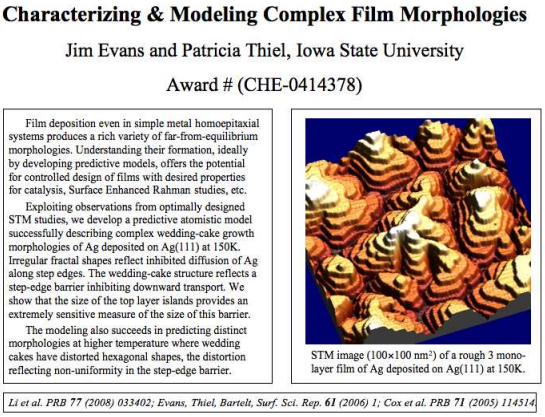

Figure 6: A picture showing Silver on Silver epitaxy from the talk by Jim Evans

also spoke about growth of Silver on Nickel/Aluminum which results in bilayers [10]. Because this system is lattice matched the bilayer are not due to strain, but instead result from the strong anisotopy between the Silver and the Nickel/Aluminium substrate.

Wei Lu. This talk was concerned with self assembly of submonolayer-thick lead films on copper [11]. He presented a continuum model that includes effects of elastic interaction and phase segregation. He showed how the different patterns form depending on the relative strength of various material parameters. He also discussed the effects of prepatterning on the final structure.

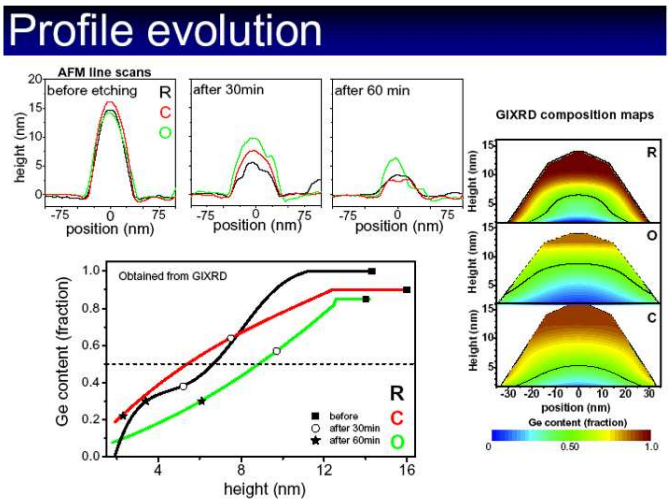

Figure 7: The morphological and compositional evolution of SiGe quantum dots, according to Medeiros-Ribeiro.

Gilberto Medeiros-Ribeiro. The thermodynamics of the composition of self-assembled quantum dots was the focus of this talk, which began with a presentation of experimental results showing detailed compositions maps of quantum dots before and after annealing [12]. The results indicated there was a noticeable difference in the compositional maps. This led to considerable discussion as to the mechanism causing the difference since several people argued that bulk diffusion should be quite small in such systems. This experimental

result points directly to the need for strong interactions between experimentalists, theorists, and simulators in order to unravel all of the mechanisms of film growth.

Vitaly Shchukin. The topic of this presentation was the importance of nanofaceting and heteroepitaxy in III-V type systems with special emphasis on electronic device manufacturing. [13] He spoke about alloy phase segregation on vicinal surfaces and discussed experimental results that show high index samples give rise to lateral composition modulation.

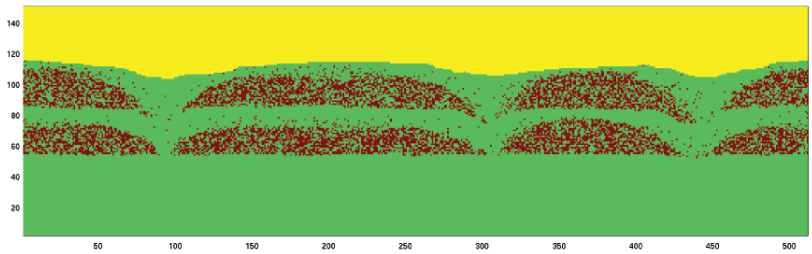

Figure 8: Simulation of stacked quantum dots from Arvind Baskaran's presentation

Arvind Baskaran. This talk was concerned with the simulation of heteroepitaxial growth using kinetic Monte Carlo. Much of the talk focused on efficient numerical methods based on the multigrid and the expanding region methods. He also presented results showing that surface segregation can lead to Stranski-Krastinov growth, as has been suggested by Cullis et al[3] and Tu and Tersoff[1]. Arvind's talk was joint work with Tim Schulze, Giovanni Russo, Jason Devita, and Peter Smereka (workshop participants). Two pertinent references for this material are [14] and [15].

Robert Kohn. Professor Kohn spoke on a variational model of faceted film evolution. He described the mathematical framework of gradient descent with respect to the H^{-1} norm [16].. The numerical implementation of such evolution equations was outlined, especially those schemes that are consistent with the gradient descent form of the equations. Finally, Professor Kohn described self similar solutions of this equation and sketched the proof of stability.

Zbig Wasilewski. The effect of defects on the fabrication of a new type of quantum well infrared GaAs/AlGaAs photodetector was discussed in this talk [17, 18]. The source of the defects was not completely understood, but evidence suggested that the defects were not threading dislocations, but maybe the result of contamination. This work shows the importance of challenging commonly held expectations in film growth, and look to other considerations to explain observed phenomena.

Ya Hong Xie. Professor Xie spoke on the dependence of surface roughening on the sign of the strain in Si-Ge systems [19]. They found that the more tensile the Si layer the smoother the resulting film, in contrast to the behavior of compressively stressed films. This result was one of the first of its kind to show that existing models, which assumed symmetry in the role of strain, were incomplete.

Giovanni Russo. Professor Russo outlined an efficient numerical technique for computing displacement fields in elastically strained thin films. The method he described was based on two ideas, the first was an artificial boundary condition which allows one to include the semi-infinite substrate[14]. The second was a multigrid method that can handle complex domains and yet take advantage of the underlying Cartesian structure[15].

Frederic Gibou. A new approach to solving partial differential equations on non-graded Cartesian grids was described by Gibou [20]. Non-graded Cartesian grids are those that allow an arbitrary level of refinement

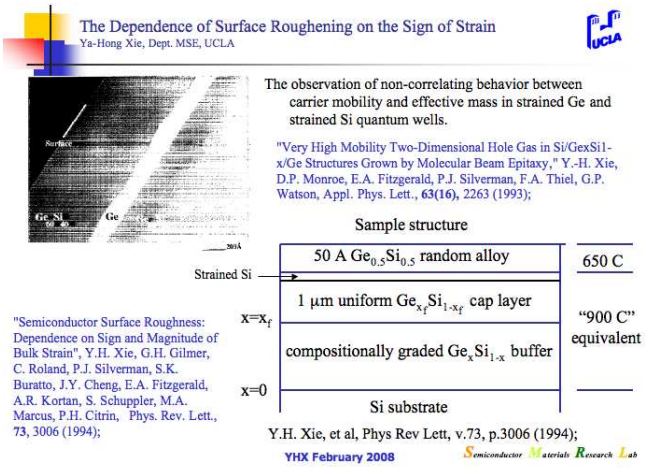

Figure 9: A slide from the talk by Ya Hong Xie that shows experimental evidence for a sign dependence on mismatch induced roughening.

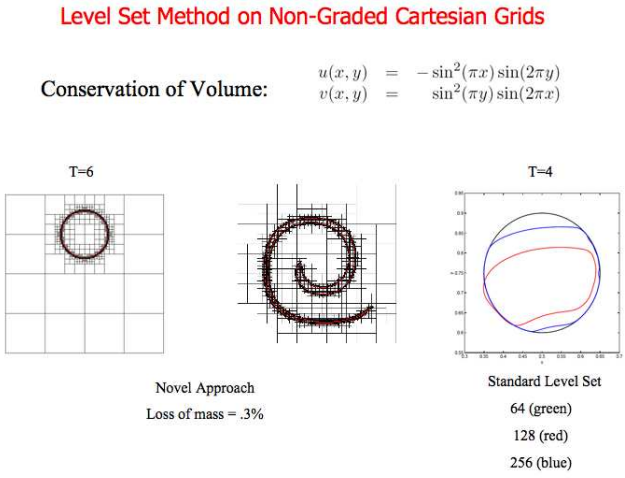

Figure 10: A slide from Frederic Gibou's talk showing a nongraded adaptive cartesion grid used for the test problem of simple advection.

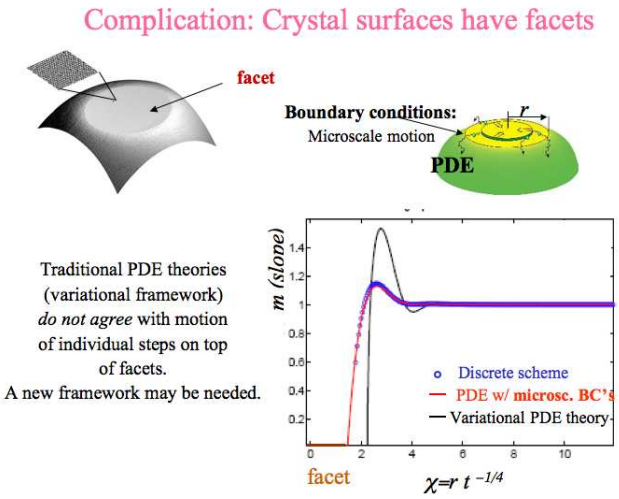

Figure 11: A slide from the talk of Dionisios Margetis

between regions. They have many advantages in terms of construction and computational efficiency. The talk concluded with several applications including crystal growth.

Dionisios Margetis. In this talk, Professor Margetis described work in which a continuum model was formulated for step motion in the presence of a facet. The main result is that microscale effects, which enter the PDE solutions via boundary conditions at facets, can affect the surface profiles macroscopically. This consideration aims at enabling predictions for the stability of nanostructures. More details can be found in Ref. [21].

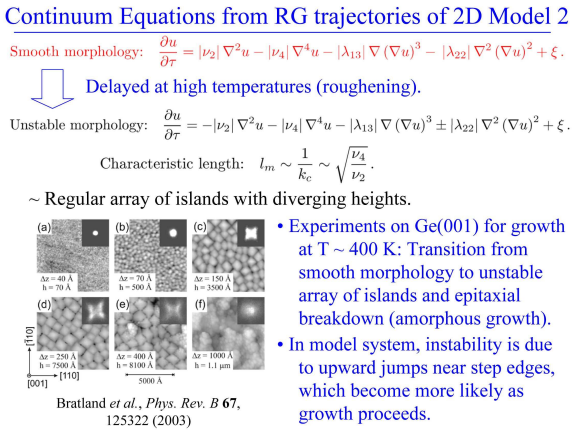

Figure 12: A summary slide from the presentation of Christoph Haselwandter

Christoph Haselwandter. This talk was concerned with the development of partial differential equations (PDE) that provide a coarse-grained description of various discrete stochastic processes. [24] Starting with the master equation of a discrete process, he outlined how one could systematically derive a PDE. The asymptotic behavior of the resulting PDE was analyzed using a renormalization group (RG) approach. This results in a set of ordinary differential equations that show the effective behavior as the system evolves.

Kristen Fichthorn. In this talk, Professor Fichthorn described algorithms to improve the computational

speed when simulating film growth using atomistic scale methods. A new approach, termed the connector model, was presented that provides a systematic approach of accounting for many body interactions. This framework was used to study hut formation of Al on Al (110) in which two, three and higher particle interactions all have comparable interactions. Also discussed was an approach based on accelerated molecular dynamics that temporally coarse-grained the fast adatom motion resulting in a more efficient algorithm. Pertinent references for this talk include Refs. [22, 23].

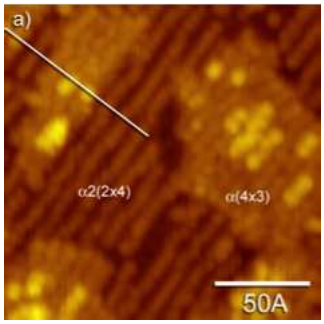

Figure 13: A figure from the talk of Jessica Bickel. It shows STM image of surface coexistence of $\alpha 2(2 \times 4)$ and $\alpha(4 \times 3)$ reconstructions in $h \sim$1.7ML Sb/GaAs(001).

Jessica Bickel. The role of strain in the surface reconstructions of III-V alloys was discussed in this talk. It was shown that in InGaAs, atomic strain due to the placement of cations induces a surface dimer ordering in the $\alpha 2(2 \times 4)$ reconstruction which is not seen in the InAs and GaAs systems. [25]. She also showed that in the GaAsSb system, lattice relaxation at step edges results in a surface coexistence of two reconstructions with the surface reconstruction coupled to the surface morphology. This was based on joint work with workshop participants Norman Modine and Joanna Mirecki Millunchick.

Axel Voigt and Dong-Hee Yeon. There were two separate talks on the phase field crystal model. In this approach, one starts with classical density functional theory and derives a model that temporally coarse-grained. The resulting phase field model requires finer that atomistic resolution in space but has the advantage of modeling on much longer time scales. As a consequence this formulation can simulate a wide range of phenomena such as elastic and plastic deformation, solidification, and grain growth. The speakers outlined both the basic ideas and the current state-of-the-art. See [26] for more details and background information.

Michael Tringides. Professor Tringides presented results in which High Resolution Electron Diffraction was used to study the growth of Lead on Silicon (111) [27]. The issue was to understand the narrow height distribution of the Lead islands. Depending on growth conditions, islands of heights 5,7, or 9 were observed. The evidence suggests that this is the result of quantum size effects, thus pointing to other mechanisms for self assembly of nanostructures.

Mark Goorsky. An entirely different technique for stacking dissimilar materials was discussed in this presentation. The basic idea was to transfer one layer to another by implanting hydrogen into the semiconductor and anneal to form blisters and induce exfoliation. [28] These blisters grow and ultimately fracture the surface and allow for placing the thin film onto a new handling wafer. While this talk was not strictly concerned with issues in heteroepitaxy, it did bring up issues relevant to defect formation and propagation.

Christian Ratsch and Xiaobin Niu. In this talk a level set formulation for island dynamics was presented. In this approach the island boundaries are iso-contours of a continuous function (the level set function). The strain and adatom fields are found by solving partial differential equations that are coupled to the islands through the level set function. Models for attachment, detachment, and nucleation are incorporated to yield the motion of island boundaries. A particular intriguing feature of this method is the fact the computational timestep can be chosen orders of magnitude larger than the timestep of typical atomic motion (diffusion).

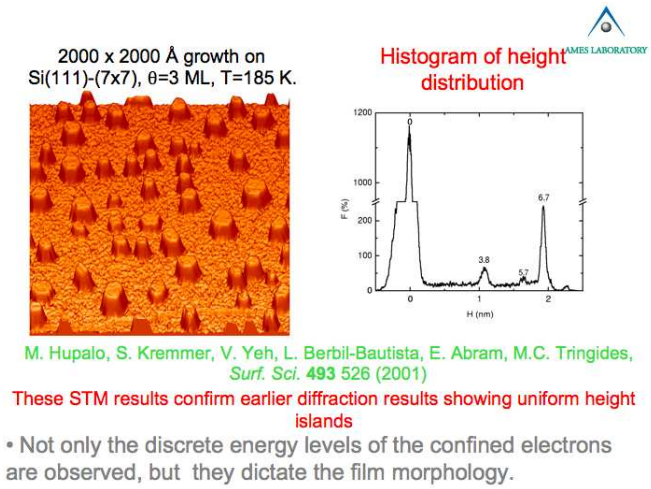

Figure 14: A slide from the talk of Michael Tringides that demonstrates quantum size effects in the growth of Lead on Si(111) films.

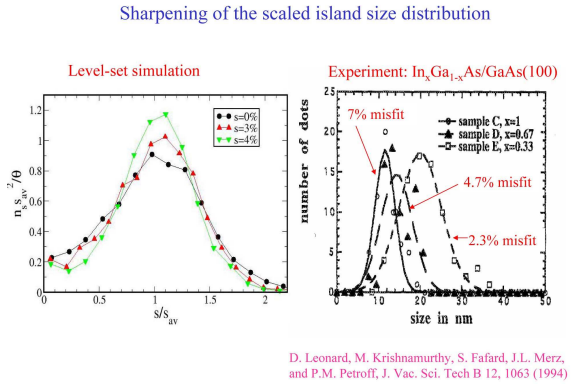

Figure 15: A slide from Christian Ratsch's talk

Therefore, it is possible to do the (expensive) calculation of the entire strain field at every computational timestep. Computed island size distribution functions are in good agreement with experiments. Some of the material presented can be found in Ref. [29]. The work presented was joint work with the workshop participants Ya-Hong Xie and Peter Smereka.

3 Outcome of the Meeting

As mentioned before, we believe that many of the outstanding problems in understanding heteroepitaxial growth can only be solved in tandem, between experimental work and modeling and computations. One immediate challenge that is well known to everyone in the community (and is often very frustrating) is the fact that experimentalists and theorist look at a problem from very different perspectives, and almost "speak a different language". It was therefore one of the main goals of this workshop to help break down this barrier, and help facilitate interactions between theorists and experimentalists. We believe that we succeeded in this respect.

The schedule was of the workshop was organized in a way that theoretical and experimental talks alternated. Most sessions were mixed. We also provided lots of time during and between talks, for many questions, and plenty of discussion. Therefore, we believe (and are supported by the feedback we got) that the environment of this workshop fostered the interactions between theorists and experimentalists. As an example, Bob Kohn (a mathematician) and Tom Tiedje (an experimentalist), who did not know each other prior to the workshop, engaged each other in long discussions during their respective talks, and for long periods of time during some of the "free time". Mike Tringides commented that he enjoyed the extensive discussions he had with Ya-Hong Xie.

Another important outcome of this conference was that some new collaborations have been formed, and that many previous collaborations got strengthened because of this workshop. Some examples of this are the following: Dionisios Margetis (Maryland) established relationships and potential collaborations with Vivek Shenoy (Brown) and Henrique Versieux (Courant, NYU). He also made contact with M. Tringides and his experiments, and expects to develop further communication with him. Moreover, he recently started a collaboration with Matthias Scheffler (FHI Berlin), and this workshop gave him a chance to strengthen this collaboration. Christian Ratsch has recently started a collaboration with Tim Schulze, comparing fast KMC schemes with levelset method. This workshop gave them a chance to deepen this collaboration, and in fact include some new aspects that have been incorporated in their first joint publication. Ratsch is also collaborating with Peter Smereka and Frederic Gibou. These 3 recently submitted a joint proposal. They plan to combine the levelset method (as developed by Ratsch and co-workers) with the efficient strain solver of Smereka and Russo, and with efficient and elegant numerical schemes to accommodate a mixed boundary condition for the diffusion equation, as proposed by Gibou. Meeting at this workshop gave them an opportunity to discuss in more detail their planed joined future work.

We also want to point out that not only the more senior participants of the workshop gave talks, but several talks were made by more junior people. For example, A. Baskaran, J. Bickel, and X. Niu are currently graduate students. C. Haselwandter and D.H. Yeon are a post-docs whereas D. Margetis and F. Gibou are assistant professors. Such exposure is important. As an example, Xioabin Niu got a chance to present some of his Ph.D. work. He is now considered for a postdoctoral position by Kristen Fichthorn, who also attended this workshop. Jessica Bickel, a student of Joanna Mirecki Millunchick, was urged to apply to the Summer School on Surface and Nanoscale Materials to be held in Spain in May 2008 and organized by Matthias Scheffler and Kristen Fichthorn. Bickel is currently a finalist for the Young Research Prize.

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