Stress Relaxation and Defect Formation in Metamorphic Buffer Layers

- Metamorphic buffer layers are thin layers with a range of lattice constants that relax the stress due to lattice mismatch in semiconductor heterostructures without degrading the crystalline quality of the active region.

- We examined the stress evolution and defect formation in these layers using a variety of monitoring and characterization techniques (Fig. 1). We have shown that different alloy compositions have a surprising effect on relaxation efficiency (Fig. 2) arising from the type of defects that nucleate at the growing surface.

BF 0$\bar{2}$2

200 nm

Figure 1: Transmission Electron Micrograph of an 820 nm thick $GaAs_{0.5}Sb_{0.5}$ relaxed layer. The primary mode of relaxation is by the injection of pure edge dislo-cations.

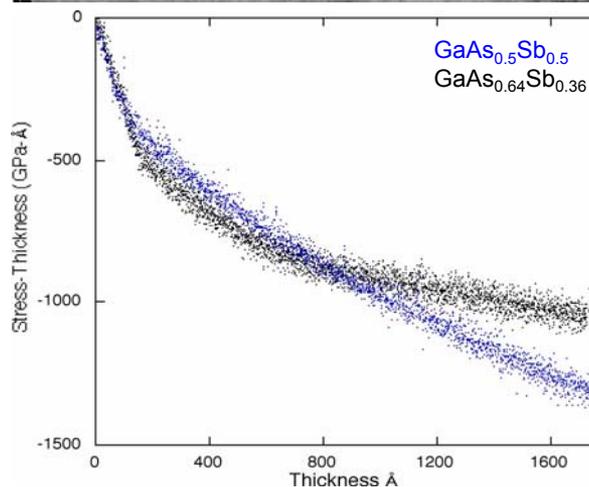$GaAs_{0.5}Sb_{0.5}$
$GaAs_{0.64}Sb_{0.36}$

Figure 2: Comparison of the Stress evolution for $GaAs_{0.5}Sb_{0.5}$ and $GaAs_{0.64}Sb_{0.36}$ showing that the less strained film relaxes at a higher rate. This is due to the nucleation of threading dislo-cations, which prop-agate through the film more readily.

A great deal of effort has been recently put into the development of High Electron Mobility Transistors (HEMTs) due to their importance in the wireless communications industry. In order to improve the device characteristics, increasing the In content in the device structure, thus the mobility*, has been of great interest. However, InGaAs, which is the most common material used in the channel of these devices, has a lattice mismatch with respect to GaAs leading to strain that can introduce mobility destroying defects. One strategy is to relax the lattice parameter in a buffer layer between the GaAs substrate and the high In-containing device structure to a value such that it can be obtained without the introduction of mobility eradicating defects. The key to the success of this approach is in the ability of the buffer layer to relax stress due to lattice mismatch without degrading the quality of the electronically active regions of the device structure.

We have investigated using GaAsSb as an alternative materials for the relaxed buffer layer. This material was chosen because it has a propensity of forming edge dislocations, which are more efficient at relieving lattice mismatch strain than the threading dislocations that form in strain-relaxed InGaAs layers. Figure 1 shows a bright field Transmission Electron Micrograph (TEM) of a $GaAs_{0.5}Sb_{0.5}$/GaAs film. The high contrast near the interface and into the film arises due to the presence of a high number of edge dislocations. By comparison, the TEM (not shown) of a $GaAs_{0.64}Sb_{0.36}$/GaAs shows a large density of threading dislocations, which are undesirable because of their ability to propagate into the channel region. Real time stress evolution was obtained using an *in situ* Multi-Beam Optical Stress Sensor (MOSS) measurement during Molecular Beam Epitaxy of these alloys (Fig.2). The *less strained film,* $GaAs_{0.64}Sb_{0.36}$/GaAs, *relaxes at a higher rate, as indicated by the steeper initial slope of the stress-thickness curve, and possesses less residual stress at the end of growth, as indicated by the greater value of the stress-thickness at high thickness. This is surprising, because one would expect that the higher strained film,* $GaAs_{0.5}Sb_{0.5}$/GaAs, would have a larger driving force for relaxation, thus a faster initial relaxation rate.

Based upon the TEM and MOSS observations, we speculate that the nucleation of threading dislocations, which are more able to glide, provide a more efficient path for strain relaxation in these films. This finding is a double edged sword, since threading dislocations also propagate into the device layers. The challenge is to create a process that activates a mechanism such that enough edge dislocations, which do not propagate, form to relieve the lattice mismatch strain

*The electron mobility in InAs is higher than that in GaAs. Therefore, InGaAs alloys has increasing electron mobilities as the In content increases.

Surface Structure of Semiconductor Alloys

- The atomic structure of compound semiconductor alloy surfaces plays an important role in the development of the final microstructure of an alloy film.

- We examine the surface structure of these alloys and have shown that their structure is significantly different than that of the individual constituents, and varies with composition (Fig.1). We have proposed a model for the most common reconstruction (Fig. 2), and shown how the coverage of each reconstruction depends on thickness (Fig. 3).
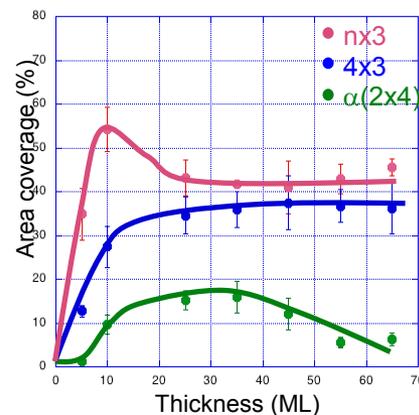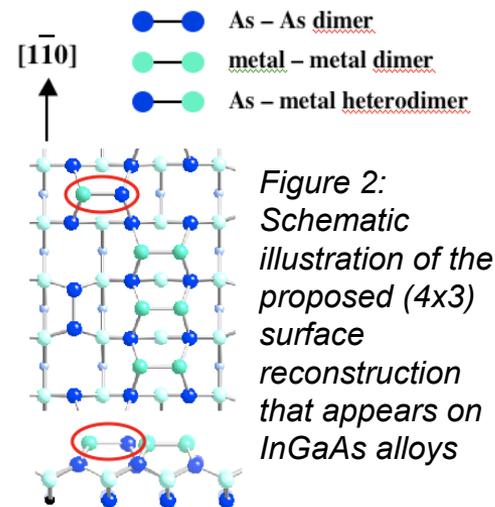
As – As dimer
metal – metal dimer
As – metal heterodimer

[1$\bar{1}$0]

Figure 2: Schematic illustration of the proposed (4x3) surface reconstruction that appears on InGaAs alloys

Figure 3: Percent coverage of each reconstruction present on a $In_{0.27}Ga_{0.73}As$ surface vs thickness.
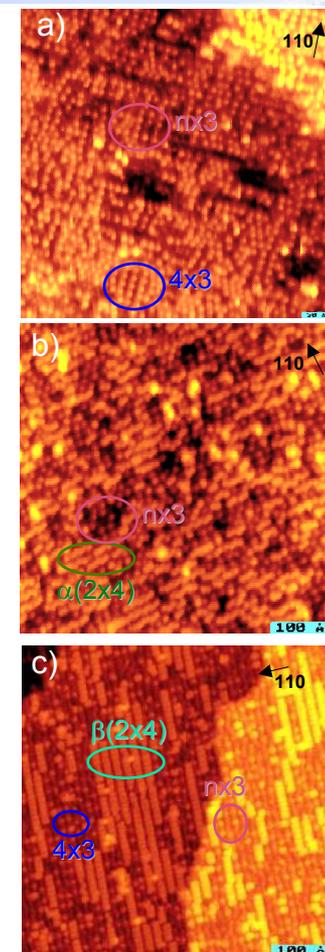

Figure 1: Scanning Tunneling Micrographs of (a) $In_{0.53}Ga_{0.47}As$ (b) $In_{0.27}Ga_{0.73}As$ (c) and $In_{0.81}Ga_{0.19}As$. Different reconstructions are indicated.

The atomic structure of compound semiconductor alloy surfaces plays an important role in the development of the final microstructure of an alloy film. Specifically, the ordering in many compound semiconductor thin films has been shown to originate from stresses induced by the surface reconstruction. In addition, interfacial broadening in device structures is thought to be related to the stoichiometry of the surface reconstruction. For In containing alloys, studies of In surface segregation suggest that the topmost layer is nearly pure InAs; however, this surface has never been imaged directly.

Despite the efforts to describe compound semiconductor surfaces such as GaAs, InAs, InP, and GaSb, the surface reconstructions of *alloy* surfaces are not well characterized. We have examined the surface structure of InGaAs alloys using a combined Molecular Beam Epitaxy and Scanning Tunneling Microscopy (STM) apparatus. We have shown that the structure of these surfaces is comprised of different reconstruction domains that depend on the surface composition and thickness of the film. From this data, a unique alloy surface reconstruction has been proposed, which is consistent with other processes that occur during growth, namely surface segregation.

The filled states (-2.3V, 100pA) STM image of a nominally lattice matched $In_{0.53}Ga_{0.47}As/InP$ surface (Fig. 1a) shows a highly disordered array of equiaxed features. Upon closer inspection, it is apparent that there is some local symmetry in the arrangement of these features. In particular, there is a reconstruction domain that possesses rectangular symmetry, with a 4a spacing along the [1 1bar 0] direction, and a 3a spacing along the [110], where a=4.1Å is the bulk lattice spacing along the <110> directions, resulting in a (4x3) reconstruction. Also apparent on the surface are more disordered regions that maintain their 3a periodicity along the [110] direction, which we refer to as the (nx3) reconstruction.

Changing the In composition significantly alters which reconstructions are present. Figure 1b is a filled state STM image (-3.11V, 100pA) of an $In_{0.27}Ga_{0.73}As/GaAs$ film. The surface exhibits equiaxed dots similar to those observed on the lattice-matched sample. The spots are not well ordered, though there is some local (4x3) symmetry apparent in the image. Approximately 15% of the surface is covered by rows aligned along the[1 1bar 0] direction that possess the zigzag character and the symmetry consistent with an $\alpha2(2x4)^*$ reconstruction typically associated with InAs(001) or GaAs(001). The surface structure is significantly different for higher In content alloys, despite the fact that the lattice mismatch is the same. Figure 1c shows an STM image of an $In_{0.81}Ga_{0.19}As/InP$ film. The surface structure is covered with various reconstructions different again from those observed on the Ga-rich surface. The most pronounced features, covering 55% of the surface, are very similar to the $\beta2(2x4)$ reconstruction observed for GaAs(001) or InAs(001). The remainder of the surface consists of both (nx3) and (4x3). It is interesting to note that the (4x3) reconstruction observed on the

$In_{0.81}Ga_{0.19}As/InP$ surface is very well organized in places.

We propose that the (nx3) and (4x3) are uniquely alloy reconstructions. Figure 2 shows the proposed model of the (4x3) reconstruction that is observed most clearly on the lattice-matched $In_{0.53}Ga_{0.47}As/InP$ (Fig. 1a). These reconstructions are unusual in that they are comprised of As dimers, metal dimers, and metal-As heterodimers. The major unit of repetition is a metal-As heterodimer resting upon an As terminated surface, with a train of metal dimers offset by a. It should be noted that there is no distinction made in this model between the metal species; thus, the metal dimers may consist of In-In, Ga-Ga, or Ga-In. InGaAs is known to order under certain growth conditions and In preferentially segregates to the surface, therefore, some specificity in metal dimer composition is likely. This model is also attractive, because it may provide an atomistic pathway for In surface segregation.

Finally, the coverages of the primary reconstruction species were measured from the STM images of the $In_{0.27}Ga_{0.73}As/GaAs$ surfaces. Figure 3 shows a plot of the area coverage of the (nx3) rows, the (4x3) reconstructions and that of the $\alpha2(2x4)$ rows with increasing film thickness, for film thicknesses < 65 ML. The coverage of the (4x3) reconstruction initially increases, and then stabilizes above 25 ML. This behavior is the same as for the variation in the surface composition with thickness, as measured by XPS (not shown). That measurement shows an initial increase in In concentration at the film surface, due to In segregation, followed by the stabilization of the surface composition at an equilibrium level. The coverage of the (nx3) and the $\alpha2(2x4)$ reconstructions also initially increases, but decreases at higher thicknesses. For the (nx3) reconstruction, this decrease is due to increasing ordering of the (nx3) as the films thickens. The decrease for the $\alpha2(2x4)$ reconstruction, however, is likely another mechanism. The initial increase in $\alpha2(2x4)$ coverage is due mostly to In enrichment of the surface due to In surface segregation, as for the (4x3). The decrease in the $\alpha2(2x4)$ coverage is accompanied by roughening of the film. Therefore, we speculate that the $\alpha2(2x4)$ is stabilized by the lattice mismatch stress. When this stress is relieved as a result of roughening, the $\alpha2(2x4)$ reconstruction is no longer stable.

This research will have a profound effect on our understanding of surface segregation and interfacial formation in compound semiconductor alloy layers, which are routinely used in device structures. We are in the process of examining these reconstructions in more detail in order to determine the atomistic mechanisms for surface segregation.

*the $\alpha2$ and $\beta2$ (2x4) reconstructions refer to different atomic arrangements that have the same (2x4) symmetry. The difference between the two arrangements is apparent in Figs. 1b and 1c.

Future Science Future Engineering, outreach to middle-school-aged girls

Activities:
- Tested microfliudic chips with different liquids
- Made glass beads
- Made ooblek and slime
- Made nail polish
- Observed the microstructure of various gels, emulsions, and foams
- Built lava lamps

Scientific and Technical concepts :
- Adhesion and wear
- Phase transitions
- Glass transition temperature
- Viscosity
- Microstructure
- Polymer structure and Crosslinking
- Microscopy
- Miscibility
- Thermal conductivity
- Thermal stress
- Electricity

Prof. Millunchick assists two girls in making glass beads

Finished beads

Lava lamps on a test run

On June 21-2, 2004, fourteen girls from area middle schools visited the departments of Materials Science and Chemical Engineering (with Prof. Mike Solomon) at the University of Michigan as a part of the Future Science Future Engineering (FSFE) Program. FSFE is a one week day program for girls who have completed the 7th or 8th grade. Each day includes hands-on laboratory experimentation, computer activities and introductions to on-line network systems. Girls meet women scientists and engineers, and obtain information about careers in science and engineering. Participants chose a special project to attend, which consists of several three-hour sessions.

The fourteen girls who came to our departments participated in several projects that demonstrate various concepts in Materials Science, Chemical Engineering, and in engineering in general. There were several basic projects. One major project was to examine and manipulate the properties of glass. First, the girls went to our glass blower's lab to see a demonstration. Next, the girls tried their own hand at glass forming by making their own decorative beads. This project allowed us to introduce the concepts of amorphous versus crystalline structure, the glass transition temperature, viscosity, and thermal stress. In order to drive these concepts even further, the girls also made ooblek and slime, discussing how the structure of the polymers (or the amount of crosslinking) affects the viscosity, etc. Finally, the girls took a tour of the MEMs lab, and tested the viscosity of various liquids an a microfluidic chip. In this way, the girls were able to connect a particular concept (how the structure of a material affects it's viscosity) using technologies ranging from the very ancient (glass making), to the modern (polymer chemistry), to the cutting edge (MEMs).

The second project was to build a lava lamp using standard materials that can be bought from a hardware store. The lava consists of a mixture of mineral oil and rubbing alcohol. At room temperature, the mineral oil is heavier than the alcohol, but as it is heated up by a lamp from below, it becomes less dense and floats to the top of the bottle. As it cools, it becomes more dense and sinks again. This allowed us to discuss the concept of miscibility and thermal conductivity. This was also the first time many of these girls have had the opportunity to wire a basic electrical device (the light bulb socket).

The third major theme was the engineering of make up. In this section, the girls made their own nail polish, while discussing the purpose of the the various ingredients (solvent, nitrocellulose, pigment) in the final product. We also talked about the properties that good nail polish should have (adhesion, wear, nontoxicity). Next, the girls took their nail polish and observed samples of it using a confocal microscope. They also looked at the structure of other personal hygiene products, such as shampoo and shaving cream. For this project, the girls learned about the science behind some of the products they use everyday. This project allowed us to further emphasize topics the addressed above, and introduced them to microscopy.

Diversity in the Mirecki Millunchick Research Group

- Top Row, left to right: Associate Professor Joanna Mirecki Millunchick, Associate Professor Chris Pearson, Jason Spalding (undergrad), Benny Perez (grad), Jenny Lee (grad)
- Bottom row, left to right: Brian Gorney (undergrad), Trey Sears (grad), Alex Riposan (grad)
- Not Shown: Jessica Bickel (grad), Darius Dixon (grad)