

## Surface Science Division Room 308 - Session SS1-TuM

### Semiconductor Surface Structure

**Moderator:** L.J. Whitman, Naval Research Laboratory

#### 8:20am SS1-TuM1 Effect of Tensile Strain on B-type Step Energy on Si(001)-(2x1) Surfaces Determined by Switch-Kink Counting, E. Heller, J.P.

Pelz, Ohio State University; D.E. Jones, Y.H. Xie, P.J. Silverman, Company  
Several years ago Xie et al.<sup>1</sup> suggested that applied strain could strongly influence the creation energy of so-called S@sub B@ steps on Si(001)-(2x1) surfaces, which could dramatically affect surface roughening during strain-layer growth. Swartzentruber et al.<sup>2</sup> and then later Zandvliet et al.<sup>3</sup> showed that step energies on unstrained Si(001)-(2x1) surfaces could be estimated by counting kinks (a kink being a small perpendicular jump in a surface step edge) on samples annealed at elevated temperatures. In order to directly test the proposal of Xie et al., we have used kink-counting in STM images of strained Si(001) surfaces to quantify the effect of strain of the S@sub B@ step energy. For this purpose, we have developed a new kink-counting method (called switch-kink counting), which is more accurate than previous methods when the azimuthal miscut angle changes across the surface. This can be problematic when there is macroscopic surface roughness, due to cross-hatch or imperfect surface preparation. I will describe both the method used by Zandvliet et al. and our new method as well as why it is more accurate for non-constant azimuthal miscut angle. I will then give an analysis of data using both of these methods on a large data set we have collected from STM images. We find an energy for these kinks that is significantly higher than that found by Zandvliet et al. for unstrained silicon, and appears to increase with increasing tensile strain, although possibly not as fast as Xie et al. predict. <sup>1</sup>Xie et al., Phys. Rev. Lett. 73, 3006 (1994). <sup>2</sup>Swartzentruber, Y.-W. Mo, R. Kariotis, M. G. Lagally, and M. B. Webb, Phys. Rev. Lett. 65, 1913 (1990). <sup>3</sup>Zandvliet, H. B. Elswijk, E. J. van Loenen, and D. Dijkamp, Phys. Rev. B, 45, 5965 (1992).

#### 8:40am SS1-TuM2 Geometry, Energetics, and Electronic Structure of the Dimer Reconstruction on the Carbon, Silicon and Germanium (100) Surfaces, H.C. Kang, C. Yang, National University of Singapore, Singapore

The ground state geometry of dimers on the C(100), Si(100) and Ge(100) surfaces have been the subject of much study and controversy, particularly in the case of the silicon surface. There are at least two issues which have not been resolved. First, theoretical calculations for Si(100) have favored both the buckled and unbuckled dimer geometry as the ground state. The most recent cluster calculations favor an unbuckled ground state while the most recent slab calculations favor a buckled ground state. Second, the driving force for dimer buckling is still not well understood. There have been suggestions that slab calculations predict the unbuckled ground state for Si(100) because of the inadequate treatment of electron correlation. We performed density functional cluster calculations for all three surfaces in an attempt to resolve these issues. We find that a number of previous cluster calculations have not dealt satisfactorily with the geometric constraints applied during geometry optimization. Our calculations resolve the differences in ground state geometry, dimer bond length and energetics between cluster and slab calculations. We also find that buckling is driven by a kinetic energy decrease, and that for silicon and germanium this dominates the increase in potential energy with buckling. For carbon the decrease in kinetic energy with buckling is less than the increase in potential energy and, hence, buckling is energetically unfavorable. We can trace this difference in behavior to the small core size of the carbon atom compared to silicon and germanium.

#### 9:00am SS1-TuM3 An Atom-Resolved Dynamical Study of Hydrogen Diffusion on the Si(100) Surface, J.J. Boland, University of North Carolina, Chapel Hill

INVITED

A detailed knowledge of the dynamical processes that occurs on surfaces has important implications for materials growth and processing. In the case of low temperature silicon growth hydrogen surface diffusion and desorption are key processes. However, little is known about the behavior of hydrogen on silicon surfaces at high temperatures. In this work we describe in detail the dynamical behavior of hydrogen on the Si(100) surface at temperatures between 600K and 750K. Our starting point for all these studies is a Si(100) surface that is completely terminated with hydrogen. At high temperatures H<sub>2</sub> desorption occurs and the dangling

bonds that result are initially localized on the same dimer unit. Even though this paired arrangement is stabilized by a weak pi interaction it soon dissociates due hopping of neighboring H atoms into these vacancy sites. Dangling bond motion is largely confined along the dimer row direction but steps act as turning points for this motion. We observe that dangling bonds recombine with surprising efficiency. A statistical analysis indicates that there are configurations other than the paired configuration that are stabilizing and that these promote dangling bond recombination. Missing dimer defects also act a recombination centers and effectively localize dangling bonds about them. Moreover, the residence times of dangling bonds at different surface locations provides a direct measure of the relative energies of the different sites on the Si(100)-2x1 surface.

#### 9:40am SS1-TuM5 Ultra-high B and As Doping during Si(001) Gas-Source Molecular Beam Epitaxy: Growth Kinetics, Dopant-Incorporation, and Electrical Activation, G. Glass, H. Kim, A. Vailionis, J. Soares, P. Desjardins, J.E. Greene, University of Illinois, Urbana-Champaign

Si(001) layers doped with B or As were grown on Si(001)2x1 substrates by gas-source molecular-beam epitaxy using Si@sub 2@H@sub 6@, B@sub 2@H@sub 6@, and AsH@sub 3@ at temperatures T@sub s@ = 500-850 °C. Dopant concentrations ranged from 1x10@sup 16@ to 1.2x10@sup 22@ cm@sup -3@ for B and 1x10@sup 16@ to 1x10@sup 18@ cm@sup -3@ for As. B incorporation was linear with incident B@sub 2@H@sub 6@/Si@sub 2@H@sub 6@ flux ratio for B concentrations C@sub B@ @<= 2.5x10@sup 20@ cm@sup -3@, and increased with higher flux ratios. As incorporation was linear to 3x10@sup 17@ cm@sup -3@, and subsequently was sub-linear. At T@sub s@ = 550 and 600 °C, B was incorporated into substitutional electrically-active sites for C@sub B@ up to 2.5x10@sup 20@ cm@sup -3@. At higher B concentrations, there is a large and discontinuous decrease in the electrically active fraction of B, although the total activated B concentration continues to increase. Hall-effect measurements show the As to be fully electrically active for all films in the study. All films were fully strained. TEM investigations revealed that B doped films grown at T@sub s@ @<= 600 °C, and all As doped films were highly perfect with no indication of precipitates or dislocations. Deuterium temperature-programmed desorption measurements as a function of increasing C@sub B@ and C@sub As@ show strong surface segregation. The B deactivation behavior can be explained on the basis of a model which accounts for strong B segregation to the second-layer, and the surface formation and subsequent incorporation of electrically inactive B-dimers at higher C@sub B@ values. In contrast, As acts to passivate the surface, resulting in arrested growth as the As coverage approaches 1 ML. The combination of HR-XRD, SIMS and Hall-effect measurements, show that the Si-B bond length due to B-dimers is 1.99 Å, compared to 2.04 Å for substitutional B atoms.

#### 10:00am SS1-TuM6 Scanning Tunneling Microscopy of B/Si(001), J.F. Nielsen, H.-J. Im, J.P. Pelz, Ohio State University; M. Krueger, B. Borovsky, E. Ganz, University of Minnesota

Previous work has shown that annealing of heavily B-doped Si(001)-(2x1) surfaces produces spontaneous formations of S@sub A@ steps into periodic "striped" patterns,<sup>1</sup> consistent with stress relaxation effects considered by Marchenko<sup>2</sup> and Alerhand et al.<sup>3</sup> However, the exact role of boron in the step formation, as well as the cause for the observed increase in step density with decreasing annealing temperature, are still under investigation. Using detailed bias-dependent STM measurements of various B-induced surface structures, we have (1) determined that the density of B-induced surface structures does NOT change significantly with annealing temperature, leaving unresolved the strong temperature dependence of the step formation, (2) observed direct evidence of boron accumulation at step edges, providing a possible mechanism for boron-induced lowering of S@sub A@-step creation energy, and (3) identified characteristic structural and electronic features of a number of distinct B-induced structures, which indicate a need to reclassify previously reported B-related structures.<sup>4</sup> We are currently introducing surface B in a controlled way by decomposing B@sub 2@H@sub 6@ on lightly P-doped Si(001). Initial observations indicate that deposition parameters determine whether B induces the formation of reconstructed islands<sup>5</sup> or whether B forms isolated structures equivalent to those observed on bulk-doped samples. Employed as a semiconductor processing step, this process could allow for the controlled production of periodic arrays of nanoscale step structures. <sup>1</sup>Pelz et al., Phys. Rev. Lett. 77, 330 (1996) <sup>2</sup>O.L. Alerhand et al, Phys. Rev. Lett. 61, 1973 (1988) <sup>3</sup>V.I. Marchenko, JETP Lett. 33, 381 (1981)

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@footnote 4@Z. Zhang et al, J. Vac. Sci. Technol. 14, 2684 (1996)  
@footnote 5@Y. Wang et al., Phys. Rev. Lett. 74, 403 (1995)

10:20am **SS1-TuM7 Halogens Adsorbed on the Ga-rich c(8x2) GaAs(001) Surface: Adsorption Sites, Mobility and Overlayer Structure**, *J.G. McLean, P. Kruse, A.C. Kummel*, University of California, San Diego

Chlorine is commonly used to etch the As-rich c(2x8) Gallium Arsenide (001) surface. However, on the well-ordered Ga-rich c(8x2) reconstruction of GaAs(001) at 300 K, Cl@sub 2@ has been found to form an overlayer which passivates the surface against attack by atmospheric gases. Although the clean surface always reconstructs, the Cl@sub 2@ passivated surface yields a sharp (1x1) LEED pattern. A more complete understanding of the Cl chemisorption is desirable both for better control of the etching process and to understand the properties of the passivating overlayer. We have used scanning tunneling microscopy to study the adsorption sites of Cl@sub 2@ on the Ga-rich c(8x2) surface of GaAs(001). The Cl bonds exclusively to the Ga atoms, consistent with expectations based on molecular bonding theory. At low coverage the Cl is mobile along the Ga rows, which is surprising given the strength of the Ga-Cl bond. We have also investigated the overlayer at high coverages, for which STM revealed both c(2x6) and (1x1) structures. In both cases, the structures are inconsistent with the Ga/As ratio of the initial clean c(8x2) reconstruction. This shows that long-range rearrangement of surface atoms has taken place, allowing a bulk terminated surface to form in the case of the (1x1) structure. Tunneling spectroscopy will be used to determine whether this surface rearrangement results in a modified electronic structure, allowing electronic as well as chemical passivation.

10:40am **SS1-TuM8 The Role of Dimer-Stacking-Fault Structures in Si(111) Etching**, *M. Fouchier, J.J. Boland*, University of North Carolina, Chapel Hill

Etching of semiconductors continues to be important from both a fundamental and applied perspective. In this work, we investigated the etching of Si(111) by halogens using Scanning Tunneling Microscopy. It is known that Si(111) etching occurs preferably at steps but also within terraces. We showed that Dimer-Stacking-fault (DS) structures are formed during etching by Bromine at 900K. These structures result from the coalescence of vacancies on the surface.@footnote 1@ These vacancies are produced either thermally or by isolate etching events. These results suggest that DS structures are intermediates in the terrace etching process and that the dimer-rows bounding these structures serve as etch sites. @FootnoteText@ @footnote 1@Marc Fouchier and John J. Boland, Phys. Rev. B 57, 8997 (1998).

11:00am **SS1-TuM9 The Structure of Ge Surfaces from (001) to (111)**, *A. Laracuente, S.C. Erwin, L.J. Whitman*, Naval Research Laboratory

We are studying the structure of Ge surfaces oriented between (001) and (111) using STM and first-principles electronic structure calculations (LDA). Similar to Si,@footnote 1@ Ge surfaces oriented within ~12° of (001) and (111) consist of low-index terraces and steps. Between this range, it appears that only (113) and ~°(559) are planar surfaces on Ge, in contrast to Si where (114), (113), and (5 5 12) are planar. Because (113) is the only planar high-index surface common to Si and Ge in this range, its structure is of particular interest. At room temperature, Si(113) has a (3x2) reconstruction that incorporates a highly unusual six-fold-coordinated surface interstitial. The "self-interstitials" occur within every other tetramer (a dimer plus nonrebonded double-layer step), making the otherwise (3x1) surface (3x2). At room temperature the Ge(113) surface consists of an equilibrium mixture of (3x1) domains (~80%) and Si-like (3x2) domains (~20%). In contrast to previously reports, we find that the (3x1) domains have the same structure as Si(113)-(3x2), with the exception that every tetramer includes an interstitial. Extensive LDA calculations confirm that the "self-interstitials" dramatically lower the surface energy on Ge(113). Whereas on Si the (3x1) structure is 2 meV/ Å@super 2@ higher in surface energy than the (3x2), it is approximately degenerate on Ge (in agreement with experiment). Furthermore, calculations of the stability of interstitials at various sub-surface sites indicate that they do not migrate to the surface from the bulk, as previously suggested, but rather originate from surface adatoms (perhaps in a lattice gas). @FootnoteText@ @footnote 1@Baski, Erwin, and Whitman, Surf. Sci. 392, 69 (1997).

11:20am **SS1-TuM10 Structure of Arsenic-Passivated Germanium (100)**, *S. Gan, L. Li, M.J. Begarney, D. Law, C. Li*, University of California, Los Angeles; *B.-K. Han*, University of California, Los Angeles, US; *R.F. Hicks*, University of California, Los Angeles

Arsenic passivation is an important first step in the heteroepitaxy of GaAs on Ge (100). Using scanning tunneling microscopy (STM), x-ray

photoelectron spectroscopy and low energy electron diffraction, we have identified the atomic structure of arsenic-terminated Ge (100) surfaces. The germanium substrates were exposed to arsenic in two different ways: (1) by dosing with 500 L arsine in ultrahigh vacuum, and (2) by exposure to 2.0 Torr tertiarybutylarsine and 97.0 Torr hydrogen at 650°C in a CVD reactor. During AsH<sub>3</sub> dosing at 25 to 300°C, the As coverage is approximately constant at 0.3 ML. Upon increasing the dosing temperature further, the coverage attains a maximum of 1.0 ML at 425°C, then gradually declines to zero at 600°C. Scanning tunneling micrographs obtained at 1 ML coverage show that the surface has been transformed into a series of flat islands, one atomic layer in height, that are terminated with arsenic dimers. Also, B-type steps are preferred over A-type steps, causing the islands to exhibit narrow rectangular shapes with long straight edges. By contrast, when the surface is treated with tertiarybutylarsine in the CVD reactor, the initial coverage of arsenic is 2.0 ML. Upon annealing these samples in vacuum, the coverage remains constant up to 300°C, then slowly drops to zero as the temperature is raised to 600°C. At more than 1.5 ML of arsenic, the As:Ge (100) surface exhibits an unusual "waffle" pattern, with ridges about 20-50 Å in width crisscrossing the surface in the [110] and [-110] directions. Heating to 425°C, decreases the coverage to 1.0 ML. In this case, the surface is terminated with a series of square, flat islands that are separated by straight step edges one to three atomic layers in height. These surfaces are completely terminated with As dimers. Further heating to desorb the arsenic, causes the Ge (100) surface to transform back into a series of large terraces with their edges composed of equal amounts of A and B steps. The unusual morphology observed after exposure to tertiarybutylarsine in the CVD reactor is attributed to hydrogen-atom etching of the germanium surface.

11:40am **SS1-TuM11 STM of Tl Overlayers on Si(111): Structures of a "New" Group III Element**, *L. Vitali, M.G. Ramsey, F.P. Netzer*, Karl-Franzens-Universität Graz, Austria

Thallium is an unusual group III element because it can adopt a monovalent state in addition to the more conventional trivalent state of the other elements of this group. In this study we investigate for the first time the growth and the structure of Tl overlayers on Si(111)7x7 surfaces from room temperature (RT) to 500°C, using STM and STS in conjunction with LEED and AES. At low coverages Tl adatoms adsorb preferentially on the faulted half of the unit cell, covering the surface with an array of triangular adsorbate islands maintaining the (7x7) periodicity. The Tl adatoms are highly mobile at RT as recognised in consecutive STM images. On completion of the first monolayer a low corrugation surface develops at RT, but at 350°C a well ordered (1x1) structure is observed in LEED and with atomic resolution in the STM. This layer shows a metallic state with a prominent feature at -0.5 eV in STS. Depending on the substrate temperature remarkable contrast phenomena are seen in the STM for the first and the second monolayer of Tl. From RT to 200°C the Si(7x7) substrate arrangement determines the structure of the overlayer, with a network of contrast lines reflecting, presumably, the (electronic?) influence of the (7x7) substrate mesh. Atomic resolution along the lines displays a different distribution of occupied and unoccupied states. From 300-450°C a (6x6) array of broad second layer maxima (~17Å diameter, corrugation ~1Å) on a (1x1) monolayer signals a structural transformation of the overlayer. Tl overlayers on Si(111) thus display a very different structural behaviour to the other group III elements and possible reasons are discussed in terms of valency, bonding geometry and size effects.

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