Chapter 5. Epitaxy and Step Structures on Semiconductor Surfaces

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5.1 Structure and Phase Behavior of the Si(113) Surface

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Recently, our efforts under JSEP have been directed towards implementation of a design for an ultra-high-vacuum (UHV) chamber for surface x-ray scattering. The design and assembly of the UHV chamber and its associated diffractometer are now complete, and a first set of experiments using the new chamber at the MIT-IBM Beamline (X20) at the National Synchrotron Light Source has been carried out.

Our initial program (in collaboration with R.J. Birgeneau) is to study the Si(113) surface.[1] Si(113) is interesting for a number of reasons, which involve both possible technological applications and interest in the basic physics of surfaces. Firstly, we note that Si(113) is a stable facet with a surface energy comparable to that of the (111) or (001) orientation.[2] Reports of superior epitaxial growth on Si(113)[3] make the structure of this surface and its temperature dependence especially worthy of study.

An unreconstructed (113) surface may be envisaged as a sequence of (001) terraces separated by (111) steps. (The terraces are a single atomic row wide.) The corresponding surface unit cell contains two different types of surface atom: two-fold coordinated atoms deriving from the (001) terrace with two dangling bonds and three-fold coordinated atoms from the (111) step with a single dangling bond (see figure 1, which is taken from the article by Myles and Jacobi[4]). As noted by others before,[5] this aspect of the (113) surface leads to the possibility of two different adsorption sites. This feature may alleviate the problem of twinning that occurs in the growth of III-V semiconductors on flat Si(001).[6] Furthermore, in a III-V material, the (113) surface is non-polar, in contrast to the (001) and (111) surfaces, which makes it especially interesting for heteroepitaxy.

The clean Si(113) surface reconstructs to form either a (1x3) or a (2x3) surface mesh. The (1x3) structure appears to be the equilibrium configuration,[7] but the precise atomic geometry of the Si(113) (1x3) reconstruction has yet to be established experimentally Moreover, convincing calculations of the structure of Si(113) do not currently exist. At elevated temperatures ($\gtrsim$840K), the surface reverts from its (1x3) structure to a structure with true (1x1) symmetry of bulk (113)

1 B.F. Olshanetsky and V.I. Mashanov, *Surf. Sci.* III: 414 (1981); D.J. Chadi, *Phys. Rev. B* 29: 785 (1984).

2 J.M. Gibson, M.L. McDonald, and F.C. Unterwald, *Phys. Rev. Lett.* 55: 1765 (1985).

3 G.H. Olsen, T.J. Zamerowski, and F.Z. Hawrylo, *J. Cryst. Growth* 59: 654 (1982); S.L. Wright, M. Inada, and H. Kroemer, *J. Vac. Sci. Technol.* 21: 534 (1982).

4 U. Myles and K. Jacobi, *Surf. Sci.* 220: 353 (1989).

5 D.J. Chadi, *Phys. Rev. B* 29: 785 (1984); U. Myles and K. Jacobi, *Surf. Sci.* 220: 353 (1989); J. Knall, J.B. Pethica, J.D. Todd, and J.H. Wilson, *Phys. Rev. Lett.* 66: 1733 (1991).

6 K. Fujikawa, *J. Cryst. Growth* 77: 509 (1986).

7 Y.N. Yang, E.D. Williams, R.L. Park, N.C. Barlett, and T.L. Einstein, *Phys. Rev. Lett.* 64: 2910 (1991).
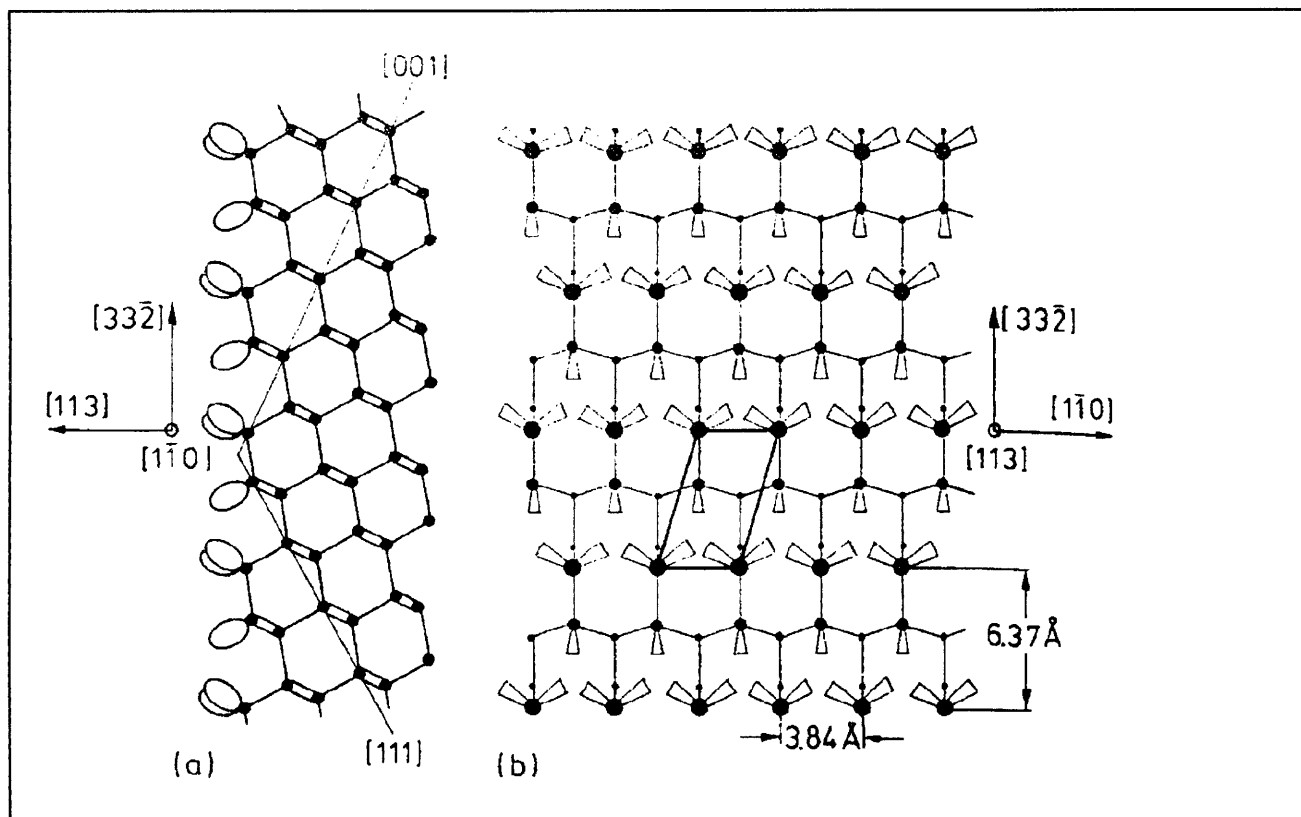
Figure 1.

planes.[7] It has been suggested that the phase transformation between these two surface configurations falls into a particular "universality class," that of the chiral, three state Potts model.[8] Our initial experiments, aimed at studying this aspect, were carried out on a (1x3) reconstructed surface, produced by annealing at 1500 K and subsequently cooling to below the (1x3)-to-(1x1) transformation temperature ($\gtrsim$840K). The presence of commensurate "1/3-order" rods, located between the rods of scattering associated with bulk periodicities, indicates a (1x3) reconstruction of the crystal surface. A scan across one such rod—the (4,2/3) rod (we employ the units of the unreconstructed surface unit cell)—is shown for several temperatures in figure 2 on a logarithmic intensity scale. The lowest profile shown corresponds to a temperature of 750 K. Evidently, the reconstruction is readily observable. In addition, the width of this profile determines that the reconstruction is translationally well-ordered on length

scales of $\cong$ 4000Å. (Other measurements establish that the existence of peaks associated with a (2x3) structure is excluded at the 10^{-4} level.) The additional profiles in figure 2 illustrate the behavior observed on warming through the phase transformation. The commensurate 1/3-order rod becomes weaker, and at the same time a broad, incommensurate peak may be seen emerging towards smaller wave vector (smaller K). Least-mean-squares fits (solid lines) reveal that the width of the incommensurate peak is proportional to its displacement from the commensurate position, suggesting that the disordering indeed falls within the universality class proposed.

Experiments to investigate the detailed atomic structure in the commensurate phase are planned for the near future. Another interesting possibility is that of surface roughening, which may occur at very high temperatures. Experiments to investigate this aspect are also forthcoming.

[8] Y.N. Yang, E.D. Williams, R.L. Park, N.C. Barlett, and T.L. Einstein, *Phys. Rev. Lett.* 64: 2910 (1991); D.A. Huse and M.E. Fisher, *Phys. Rev. B* 29: 239 (1984).
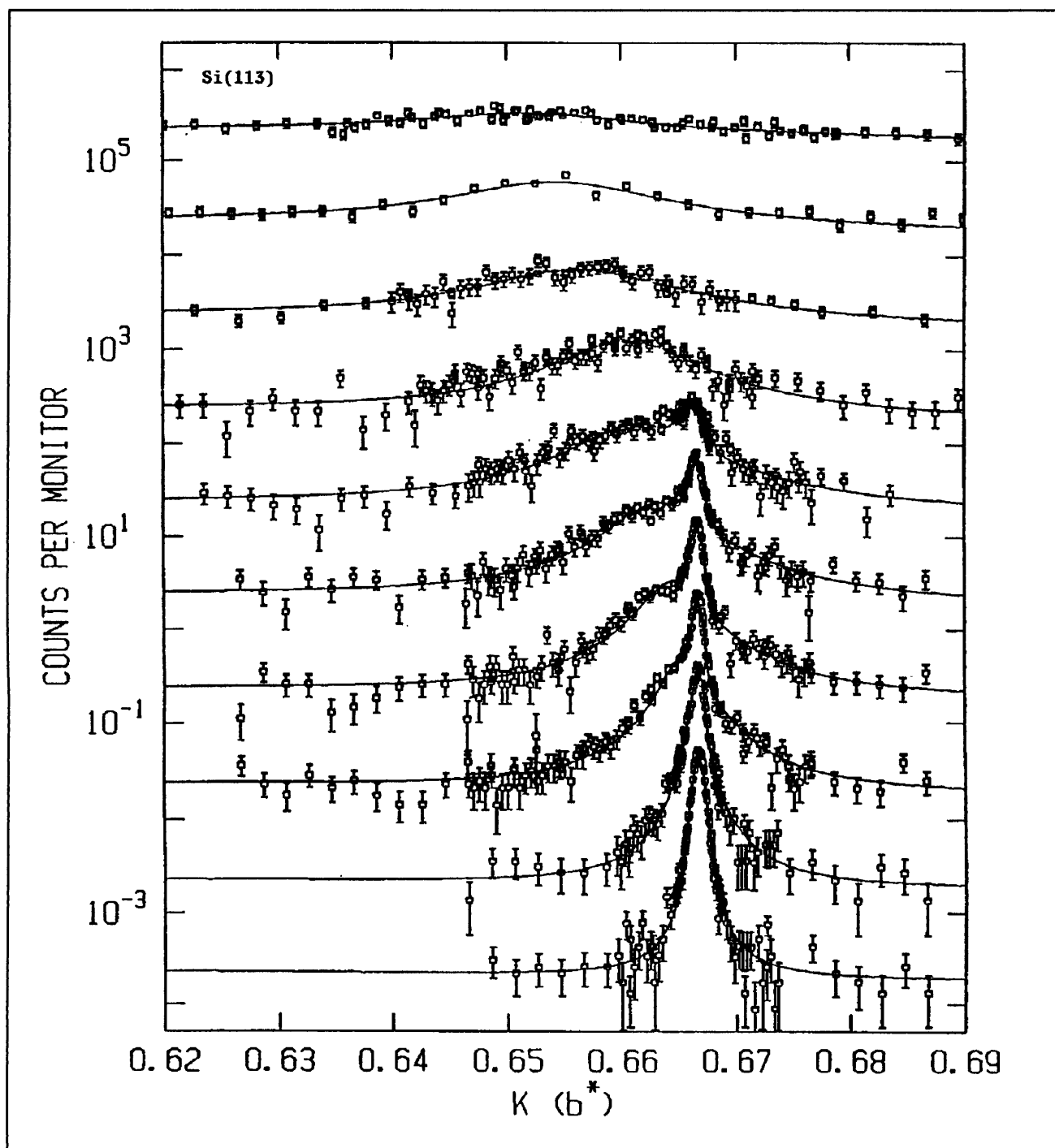
Figure 2.

Publications

Abernathy, D.L., S.G.J. Mochrie, D.M. Zehner, G. Grübel, and D. Gibbs. "Orientational Epitaxy and Lateral Structure of the Hexagonally Reconstructed Pt(001) and Au(001) Surfaces." *Phys. Rev. B* 45 (1992). Forthcoming.

Gibbs, D., G. Grübel, D.M. Zehner, D.L. Abernathy, and S.G.J. Mochrie. "Orientational Epitaxy of the Hexagonally Reconstructed Pt(001) Surface." *Phys. Rev. Lett.* 67: 3117 (1991).