

Chapter 5. Epitaxy and Step Structures on Semiconductor Surfaces

Academic and Research Staff

Professor Simon G.J. Mochrie

Graduate Students

Douglas L. Abernathy

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

Sponsor

Joint Services Electronics Program
Contract DAAL03-92-C-0001

Over the last year, we have pursued a comprehensive x-ray scattering study of the structure and phase behavior of the Si(113) surface in collaboration with Professor R.J. Birgeneau. The results will allow us to determine the atomic structure of the (3×1) reconstructed Si(113) surface. Moreover, it is already clear that our results represent an important advance for our basic understanding of order-disorder transformations in model two-dimensional systems.

In theoretical models of an overlayer on a substrate, it is possible to identify four generic phases. (1) Commensurate (C) solids are characterized by long-range translational order and a wavevector which is commensurate with the substrate lattice. (2) C-fluids are also characterized by a commensurate wavevector, but their translational correlation length is finite. (3) Incommensurate (IC) floating solids exhibit a wavevector which is incommensurate with the substrate and an infinite correlation length. (4) Finally, IC-fluids show an incommensurate wavevector and a finite correlation length.

The critical behavior at the phase transformations between these different structures is largely known: C-solid-to-fluid transformations are described by p -state Potts models, where p is the order of the commensurability (which is defined as the period of the overlayer measured in units of the substrate lattice constant).¹ IC-solid-to-fluid melting is Kosterlitz-Thouless melting.² The transformation between a C-solid and an IC-solid is a Pokrovski-Talapov transformation for uniaxial phases³ and discontinuous in the hexagonal case.⁴ C-fluids and IC-fluids are separated by so-called disorder lines.⁵

Each of the above mentioned transformations is well understood theoretically. The situation is more complicated for the transformation from a C-solid into an IC-fluid, where the order of the commensurability (p) is key in determining the expected behavior. For $p \geq 4$, there is general agreement that an IC-solid phase always separates the C-solid and IC-fluid phases. For $p=2$, there is agreement that near the critical temperature for the C-solid-to-IC-fluid transformation the correlation length, incommensurability, susceptibility, and order parameter show power-law behavior. This behavior is characterized by the same critical exponents ($\nu, \bar{\beta}, \gamma, \beta$, respectively) as found for the C-solid-to-fluid transformation, i.e., the universality class of the transformation is that of the 2-state Potts model. In contrast, for $p=3$ the character of the transformation from a C-solid into an IC-fluid phase remains unresolved. There are three possible scenarios. The first is that a direct C-solid-to-IC-fluid transformation cannot occur;

¹ M. Schick, *Surf. Sci.* 11: 245 (1981).

² J.M. Kosterlitz and D.J. Thouless, *J. Phys. C* 6: 1181 (1973).

³ V.L. Pokrovski and A.L. Talapov, *Phys. Rev. Lett.* 42: 65 (1979).

⁴ J. Villain, *Surf. Sci.* 97: 219 (1980).

⁵ V.J. Emery and I. Peschel, *Z. Phys. B* 43: 241 (1981).

instead, an IC-solid phase inevitably intervenes.⁶ The second possibility is that there is a direct transformation, which falls in the same universality class as the C-solid-to-fluid transformation (3-state Potts universality class).⁷ Finally, Huse and Fisher⁸ have suggested that there may be a direct transformation, but that it is in a new *chiral melting* universality class, with as-yet-unknown critical exponents.

The signature of a chiral transformation is that the product of the incommensurability and the correlation length approaches a constant near the critical temperature (T_c), i.e., $\bar{\beta} = v$.⁸ In contrast, according to den Nijs, the product of the incommensurability and the correlation length goes to zero near T_c . Specifically, he predicts $\bar{\beta} = 2v$. It is clear that careful studies of experimental realizations of a system such as the Si(113) surface, which determine critical behavior, are particularly valuable. Below $T_c = 959$ K, Si(113) exhibits a (3×1) commensurate reconstruction ($p=3$) and a transformation into a disordered IC structure for temperatures above T_c .⁹ For Si(113), the reconstructed surface layer plays the role of the overlayer, while subsequent layers with bulk periodicity constitute the substrate.

Figures 1 and 2 show x-ray diffraction profiles obtained at the National Synchrotron Light Source near the surface $(5/3, 1)$ position in reciprocal space for several different temperatures. This experiment employed our new JSEP-funded UHV surface x-ray scattering apparatus. Below T_c the scattering profile consists of a narrow profile located at the $(5/3, 1)$ -position ($\sigma = \tau = 0$). For temperatures increasing above T_c , the peak of the scattering shifts away from $\sigma = 0$ (y-direction) and broadens in both σ and in τ (x-direction). The peak shift reflects the formation of discommensurations in the erstwhile commensurate reconstruction, so that the surface layer is now incommensurate. The peak broadening indicates that the translational correlation length in the incommensurate phase is finite, i.e., it is an IC-fluid. Figure 3 shows results for the dependence of the incommensurability (ϵ), the inverse correlation lengths (κ_y and κ_x), the square of the order parameter (I_0), and the wavevector dependent susceptibility (χ) versus reduced temperature $((T - T_c)/T_c)$.

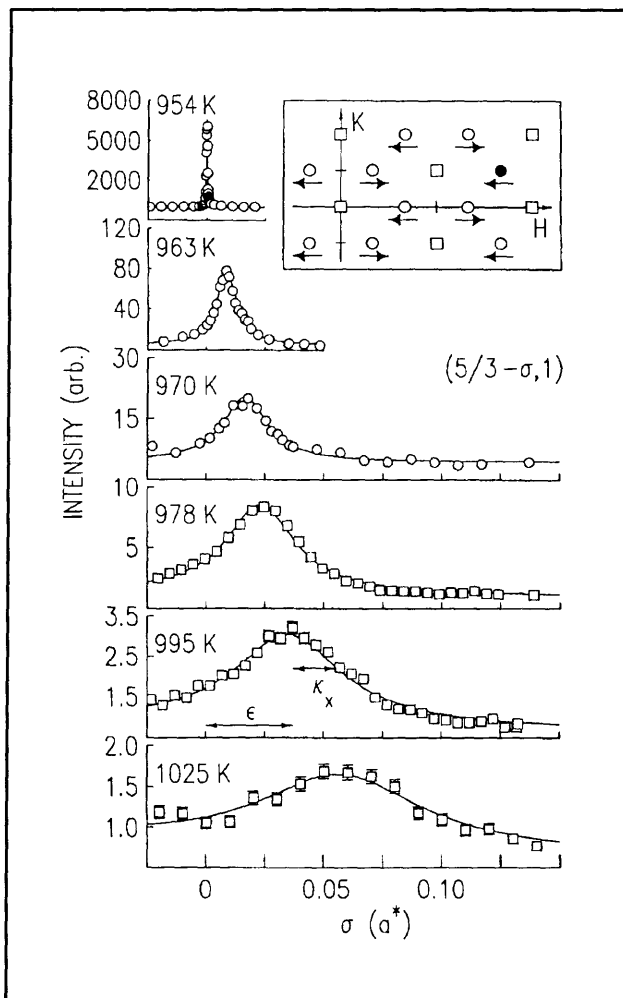


Figure 1. Scans along the x-direction through the $(5/3, 1)$ position in the reciprocal space of the reconstructed Si(113) surface versus temperature. The solid lines are least-mean-squares fits of a Lorentzian scattering function plus a smoothly-varying background to the data, which determine the peak shift from the commensurate position, i.e., incommensurability (ϵ), peak width (κ_x) and peak intensity (χ).

Each of these quantities shows power-law behavior over approximately two decades of reduced temperature with exponents $\bar{\beta} = 0.63 \pm 0.05$ for the incommensurability, $v_x = 0.65 \pm 0.07$ for the inverse correlation length in the incommensurate direction,

⁶ F.D.M. Haldane, P. Bak, and T. Bohr, *Phys. Rev. B* 28: 2743 (1983).

⁷ S.F. Howes, *Phys. Rev. B* 27: 1762 (1983); M. den Nijs, *Phase Transitions and Critical Phenomena*, eds. C. Domb and J. Lebowitz (London: Academic Press, 1987).

⁸ D.A. Huse, and M.E. Fisher, *Phys. Rev. Lett.* 49: 793 (1982).

⁹ Y.N. Yang, E.D. Williams, R.L. Park, N.C. Bartelt, and T.L. Einstein, *Phys. Rev. Lett.* 64: 2410 (1990); B.Z. Olshanetsky and V.I. Mashanov, *Surf. Sci.* 111: 414 (1981).

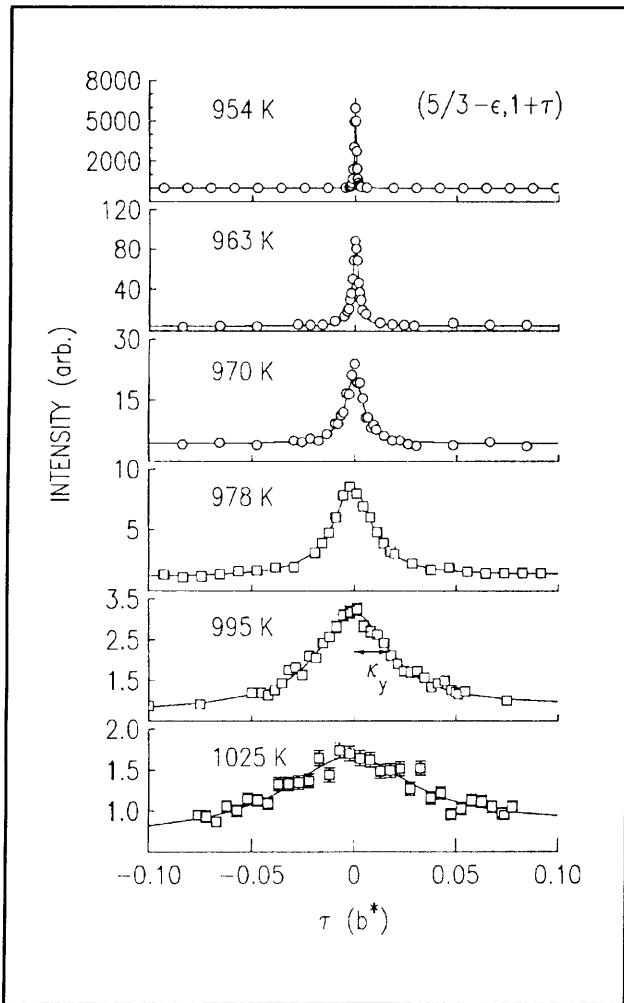


Figure 2. Scans along the y -direction through the $(5/3-\epsilon, 1)$ position in the reciprocal space of the reconstructed Si(113) surface versus temperature. The solid lines are least-mean-squares fits of a Lorentzian scattering function plus a smoothly varying background to the data, which determine peak width (κ_y), and peak intensity.

$\nu_y = 1.05 \pm 0.07$ for the inverse correlation length in the transverse direction, $2\beta = 0.23 \pm 0.03$ for the square of the order parameter, and $\gamma = 1.56 \pm 0.10$ for the susceptibility.

These results are striking for several reasons. First, we believe that the data presented in figures 1, 2, and 3 represent the highest quality measurements to date of surface critical exponents. The results are particularly impressive when one considers that the scattering emanates from relatively high-index Si surface and that Si is not a strong

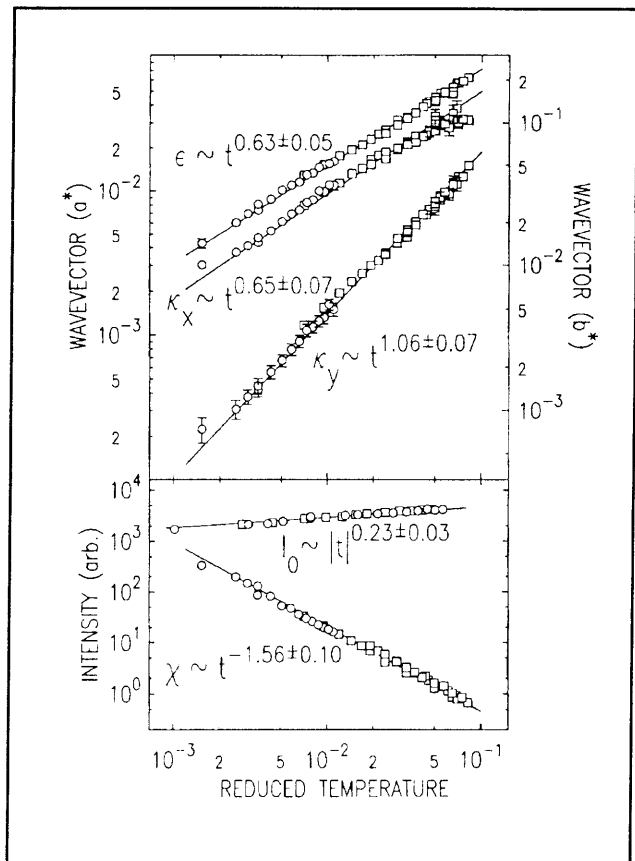


Figure 3. Dependence of the incommensurability (ϵ), inverse correlation lengths (κ_x and κ_y), susceptibility (χ), and square of the order parameter (I_0) versus reduced temperature ($(T - T_c)/T_c$). Note the log-log scales.

x-ray scatterer. They demonstrate that our apparatus teamed with an intense synchrotron x-ray source constitutes the world's premier facility for surface x-ray diffraction studies. Only with such high quality data is it possible to accurately determine critical exponents. Second, it is clear that the exponent for the correlation length along the x -direction is different from that for the correlation length along the y -direction, i.e., there is *anisotropic scaling*. Such behavior is unusual, although one instance in which it occurs is the uniaxial C-solid-to-IC-solid transformation, where exact results give $\nu_x = \beta = 1/2$ and $\nu_y = 1$.¹⁰ Furthermore, Howes¹¹ has suggested that $\nu_y = 1$ and $\nu_x = 2/3$ at the special point in the phase diagram (Lifshitz point) where the line of direct C-solid-to-IC-fluid transformations ends and is replaced by successive C-solid-to-IC-solid and IC-solid-to-IC-fluid transformations. Third, the measured exponent values are

¹⁰ V.L. Pokrovski, and A.L. Talapov, *Phys. Rev. Lett.* 42: 65 (1979).

¹¹ S.F. Howes, *Phys. Rev. B* 27: 1762 (1983).

consistent with the hyperscaling relation: $\nu_x + \nu_y = \gamma + 2\beta$. A final important observation is that the product of the incommensurability and the correlation length along the incommensurate direction is constant ($\beta = \nu_x$) as expected for chiral melting.

A direct C-solid-to-IC-fluid transformation indicates that the phase diagram proposed by Haldane et al. is incorrect. Furthermore, the observation of anisotropic scaling informs us that the disordering transformation of Si(113) is not in the universality class of the 3-state Potts model. It follows that these data imply that the C-solid-to-IC-fluid transformation of Si(113) lies in a chiral melting universality class as proposed by Huse and Fisher. Moreover, the previously unknown exponents which characterize the chiral melting universality class have been determined.

We are confident that these results will stimulate and guide further theoretical work aimed at finally

understanding the critical behavior at the C-solid-to-IC-fluid transformation with $p=3$. This would complete our understanding of phase transformations in this type of *model* two-dimensional system.

5.2 Publications

Abernathy, D.L., S.G.J. Mochrie, D.M. Zehner, G. Grübel, and D. Gibbs. "Thermal Roughness of a Close-Packed Metal Surface: Pt(001)." *Phys. Rev. Lett.* 69: 941 (1992).

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) Surface." *Phys. Rev. B* 45: 9272 (1992).