Chapter 6. Epitaxy and Step Structures on Semiconductor Surfaces

Academic and Research Staff

Professor Simon G.J. Mochrie

Graduate Student

Douglas A. Abernathy

6.1 Project Description

Sponsor

Joint Services Electronics Program
  Contract DAAL03-89-C-0001

Under the Joint Services Electronics Program, we have studied the Pt(001) surface as a model for the behavior of an incommensurate overlayer on a substrate.[1] This research will lead to a more complete understanding of what determines the orientation of a thin film on a substrate.

The (001) surface of platinum, like the (001) surfaces of gold and iridium, exhibits a radical reconstruction in which the topmost layer of atoms forms a hexagonal layer, in spite of the layers of square symmetry beneath. At T = 300 K, the hexagonal overlayer is rotated by 0.75 degrees away from a high symmetry direction of the cubic lattice (the substrate). Our recent synchrotron x-ray measurements have revealed, however, that the overlayer experiences a completely new class of rotational transition at high temperatures. For T > 1670 K, the hexagonal overlayer is aligned with the cubic substrate. The temperature $T_c = 1670$ K marks the onset of rotation, and as the temperature decreases further the rotation angle increases continuously, reaching 0.75° at T = 1300K. Figure 1 shows typical experimental profiles. The two peaks are arranged symmetrically about the high symmetry [1, 1, 0] direction and correspond to positive and negative rotation angles of the overlayer. The accompanying change in the overlayer lattice constant is on the order of one part in 1000.

Current theories of orientational epitaxy predict a definite relationship between the overlayer lattice constant and the rotation angle,[2] but our observations contradict this understanding. Nevertheless, the evolution of rotation angle with temperature follows a power-law behavior (see figure 2). In fact, the observed exponent is one-half, indicative of so-called mean-field behavior. An exponent of one-half is unusual for a two-dimensional phase transition because the effect of fluctuations are expected to be particularly severe in two-dimensions. However, an elegant interpretation is possible: If one supposes that the rotational transition occurs as a result of a rotational elastic constant becoming zero, then by considering the effect of such behavior on the low-energy modes (lattice vibrations) of the Pt overlayer, it emerges that there is no mode that becomes soft as the transition is approached. In other words, there simply are no fluctuations, and character of the transition must be mean-field.[3] With this observation, we can

[1] D.L. Abernathy, S.G.J. Mochrie, D.M. Zehner, G. Grübel, and D. Gibbs, "Rotational Transitions of the Pt(001) Surface," unpublished.; D. Gibbs, G. Grübel, D.M. Zehner, D.L. Abernathy, and S.G.J. Mochrie, "Phase Behavior of the Pt(001) Surface: X-Ray Measurements," unpublished.

[2] J.P. McTague and A.D. Novaco, *Phys. Rev. B* 19: 5299 (1979); J. Villain, *Phys. Rev. Lett.* 41:36 (1978); H. Shiba, *J. Phys. Soc. Jap.* 46:1852 (1979), 48:211 (1980).

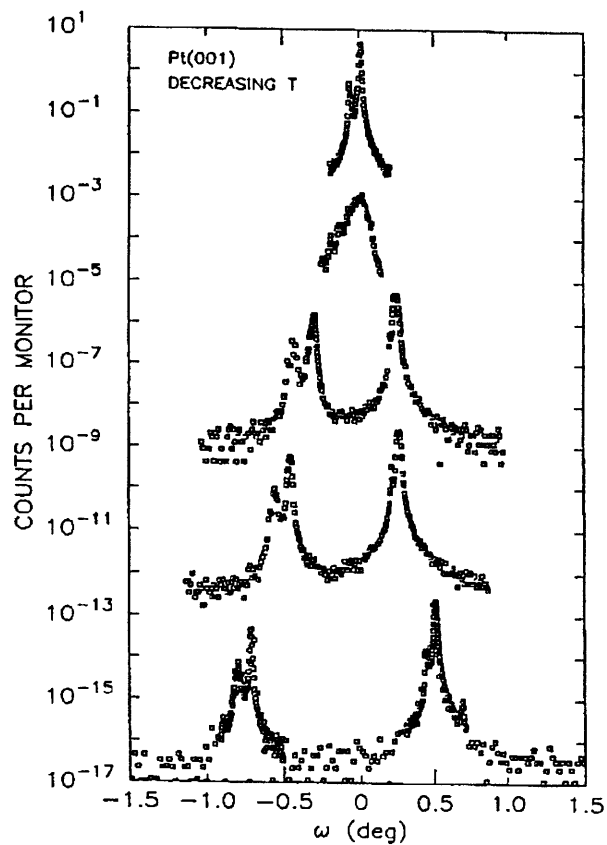[3] R.A. Cowley, *Phys. Rev. B* 13: 4877 (1976).

Figure 1. Transverse scans through a near hexagonal peak of the reconstructed Pt(001) surface for temperatures decreasing from the aligned phase (single peak) into the rotated phase (two peaks).

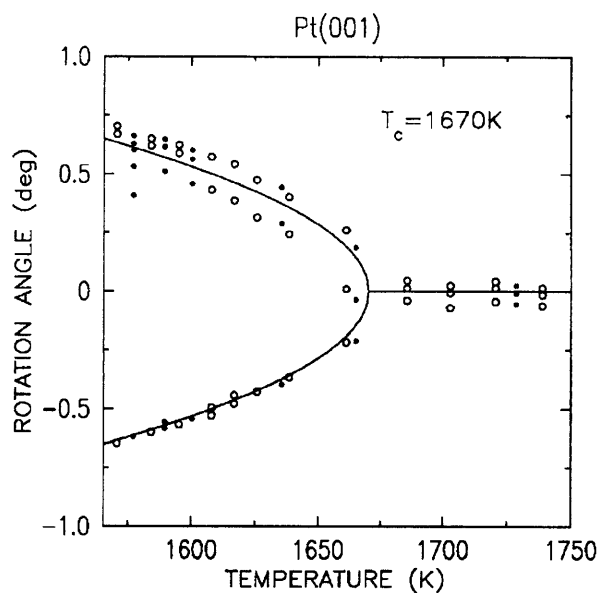also understand the mean-field character of other high temperature rotational transitions.[4]

Figure 2. Evolution of the rotation angle vs. temperature for the Pt(001) surface.

---

[4] K.L. D'Amico, D.E. Moncton, E.D. Specht, R.J. Birgeneau, S.E. Nagler and P.M. Horn, *Phys. Rev. Lett.* 53: 2250 (1984).