

# Chapter 6. Epitaxy and Step Structures on Semiconductor Surfaces

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## 6.1 Project Description

### Sponsor

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Under JSEP sponsorship, we have completed a comprehensive x-ray scattering study of the clean Pt(001) surface between 300 and 2000 K. We initiated work on this surface because it is relatively inert and detailed measurements are straightforward. However, the behavior of the Pt(001) surface has proven to be so rich that we decided a comprehensive study was mandated. Specifically, within the context of this single surface, we have obtained results that are important for understanding orientational epitaxy and associated two-dimensional phase transformations and for demonstrating that surface strain is the origin of surface reconstruction for certain metal surfaces.<sup>1</sup> Most recently, we have conducted a detailed study of the diffuse scattering in a high temperature disordered phase of this surface.

Below 1820 K, the Pt(001) surface layer exhibits a hexagonal atomic arrangement despite the planes of square symmetry which lie immediately beneath. However, above 1820 K our experiments on the Pt(001) surface reveal that there is no scattering at wave vectors associated with the hexagonal reconstruction. To elucidate the nature of the surface in this temperature range, we have performed measurements of the specular x-ray reflectivity at temperatures both above and below 1820 K. Such measurements are sensitive to the surface morphology, in particular, to surface steps

and their distribution. Simply stated, if the surface is atomically flat, the x rays are reflected only at an angle of reflection equal to their angle of incidence. On the other hand, for a surface that is not ideally flat, there is a distribution of reflected angles representative of the surface roughness. It is remarkable that the roughness of a solid surface in equilibrium is expected to result from capillary modes, just as for a liquid surface. Microscopically, the capillary modes in question are fluctuations in the location of atomic steps and islands on the surface.<sup>2</sup>

Above 1820 K, we indeed find that the distribution of reflected x rays is characteristic of a rough interface, which supports capillary modes. Our observations are important for several reasons. First, they demonstrate for the first time that close-packed surfaces, in this case, fcc(001), may become rough at temperatures below the bulk melting point. Second, detailed analysis of the distribution of reflected x rays, as the angle of incidence is varied, provide the most compelling evidence to date that the character of the roughness is as expected. Specifically, at a given value of the momentum transfer normal to the surface ( $Q_z$ ), one expects the distribution of x rays scattered away from the specular direction to be given by<sup>3</sup>

$$I_s \sim Q_x^{-2+\eta},$$

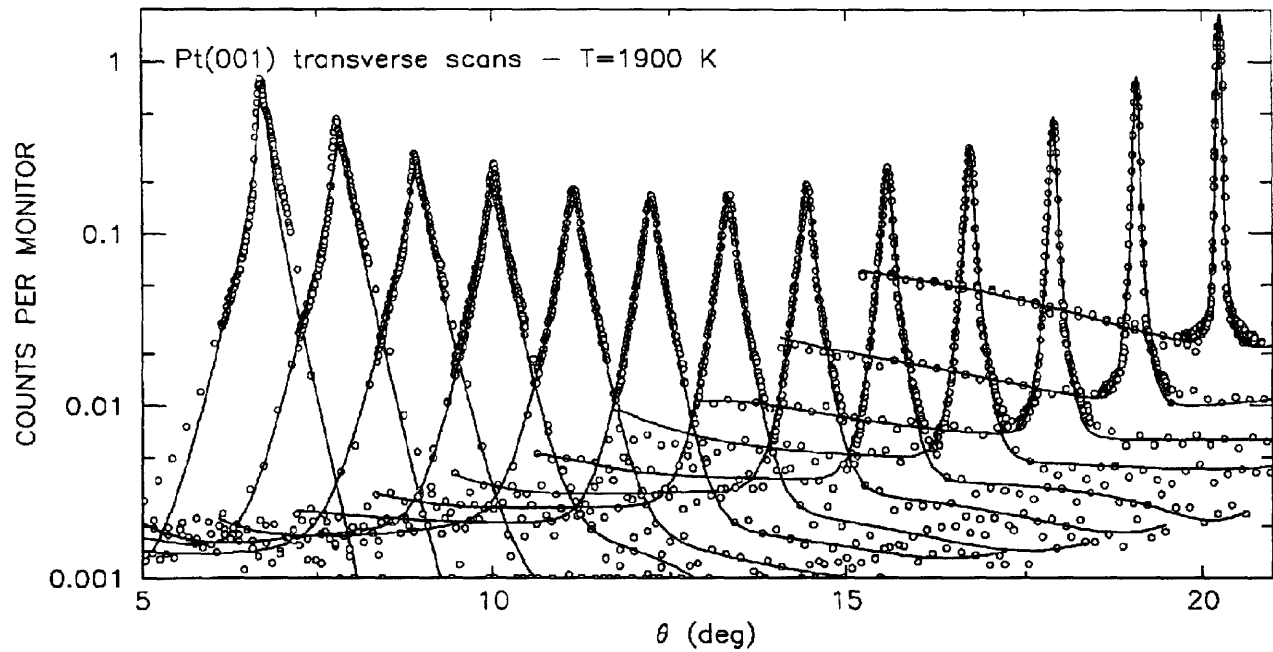
where  $Q_x$  is the deviation in wave vector from the specular condition (i.e.,  $Q_x = 0$ ). The exponent  $\eta = k_B T Q_z^2 / 2\pi\phi$ , where  $\phi$  is the surface stiffness.

<sup>1</sup> R.J. Needs, "Calculations of the Surface Stress Tensor at Aluminum (111) and (110) Surfaces," *Phys. Rev. Lett.* 58: 53 (1987).

<sup>2</sup> J.D. Weeks, "The Roughening Transition," in *Ordering in Strongly Fluctuating Condensed Matter Systems* (New York: Plenum, 1980).

<sup>3</sup> B.M. Ocko and S.G.J. Mochrie, "Facetting of the Cu(110) Surface: X-ray Fresnel Reflectivity," *Phys. Rev. B* 38: 7378 (1988).

Our results confirm, for the first time, the scaling of  $\eta$  with  $Q_z^2$ . Representative experimental profiles and the associated best fit model line shapes are shown in figure 1.



**Figure 1.** Scans across the x-ray specular reflectivity of the Pt(001) surface at different values of  $Q_z = 4K \sin \Theta / \lambda$  for  $T = 1900$  K. The solid lines show the best fit to the form discussed in the text. The fits confirm the expected scaling of  $\eta$  with  $Q_z^2$ .