11-Surfaces, Interfaces and Thin Films

Recently, we have studied the surface order-disorder transition of Cu₄Au(001) using grazing incidence x-ray diffraction [1]. Detailed surface x-ray truncation rod scans reveal novel surface ordering phenomena. In this presentation, we will discuss the analysis of the rod intensity based on a modified dynamical theory. The wavefields are derived in a form which can be treated as decoupled refraction modes characterized by Fresnel's coefficients. The corresponding dispersion surface is analytically constructed from the Bragg law and Snell law in k-space so that the geometric picture of surface-normal scan is readily described. Using this formulation, the calculated (100)-(101) rod profile of Cu₄Au in the order phase agrees with the experimental ones. Problems in the calculation for the disordered phase will be discussed.


MS-11.01.05 Phase Transformations on Stepped Surfaces:
Chiral Melting of Si(111)* and Facetting of Miscut Pt(001)*
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Two x-ray scattering experiments carried out on stepped surfaces – Si(111) and miscut Pt(001) – will be described.

(i) Theoretical models describe that they understand continuous phase transformations in two-dimensions. The exception is the disordering of a 3-fold commensurate rodsolid in an amorphous phase. The (3 x 1)-to-disordered transition of the Si(111) surface provides an experimental realization of such a transformation. Our results provide a detailed characterization of the critical behavior, including the observation of anisotropic melting, which any complete theory of two-dimensional phase transition must be able to explain.

(ii) What happens to a stepped surface at elevated temperatures? One striking phenomenon that may occur is faceting, in that the distribution of steps is no longer uniform across the surface; instead the surface separates into highly stepped regions and flat step regions. Faceting is analogous to the phase separation of a binary liquid mixture. Our recent experiments revealed that stepped Pt(001) surfaces show reversible faceting transformations. Above T = 150 K, the steps are uniformly distributed. Between T = 150 and T = 160 K, the surface is composed of smooth, macroscopic-recrystallized regions, together with rough, stepped, unrecrystallized regions. The step separation varies as (T - Tc)/Tc0.37 consistent with a simple theoretical idea. Below 150 K, the step separation remains fixed, whereas there is no secondary faceting. At the second faceting transition, the step separation jumps to 60 Å while at the same time the stepped surface restructures.

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MS-11.01.06 APPLICATIONS OF X-RAY SCATTERING TECHNIQUES FOR THE STUDY OF ELECTROCHEMICAL INTERFACE.

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A brief description of the theory and practice of synchrotron x-ray scattering technique will be presented with emphasis on the unique characteristics of this technique that make possible the in situ structural examination of solid interfaces buried under a layer of solution; and some recent applications of the technique will be reviewed for the investigation of electrochemical interfaces. The examples will include: (1) structural studies of under-potential-deposited monolayers, (2) studies of surface reconstruction of gold single crystals, (3) study of electrochemical passive film formation at the copper/solution interface, and (4) study of structural changes of Pt(111) single crystal surface associated with incipient oxidation and reduction. In the latter work, it was shown that lifting of Pt atoms occurred, and this result substantiated the long-standing hypothesis for the place-exchange mechanism of oxidation of metal/solution interfaces. It was found that if the amount of charge transferred during the oxidation did not exceed 1.5 e/atom, the initial flat surface could be completely recovered after reduction of the oxide. While, if more charge was transferred during oxidation (up to 3.5 e/atom measured from hydrogen evolution), the top layer of the surface was irreversibly roughened.

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