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THE SURFACE RECONSTRUCTIONS OF THE (100) CRYSTAL FACES OF IRIDIUM, PLATINUM AND GOLD

I. Experimental observations and possible structural models

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The structures of the reconstructed Ir(100), Pt(100) and Au(100) surfaces have been investigated. Low energy electron diffraction (LEED) patterns are analyzed and LEED intensity versus energy data are measured. A variety of structures is observed by LEED: Ir(100) exhibits a relatively simple (1 × 5) pattern; Pt(100) shows a series of closely related patterns, a typical representative of which has a $\begin{pmatrix} 14 & 1 \\ -1 & 5 \end{pmatrix}$ structure; Au(100) usually exhibits a c(26 × 68) pattern, often inaccurately described in the literature as a (20 × 5) pattern. The reconstruction of Au(111) is also considered for comparison. Various plausible structural models are discussed, while laser simulation is used to lessen the number of these models. The analysis is completed in a companion paper where LEED intensity calculations are reported to determine the atomic locations.

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II. Structural determination by LEED intensity analysis

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The investigation, in a companion paper, of the reconstructions of the Ir(100), Pt(100), and Au(100) crystal surfaces is completed here with an extensive analysis of low energy electron diffraction (LEED) intensities, using dynamical (multiple scattering) calculations. It is found that a hexagonal rearrangement of the top monolayer is a likely explanation of the surface reconstruction. At least for Ir and Pt (no calculations were made for Au), this hexagonal layer would have a registry involving bridge sites on the next square unit cell metal layer and it is contracted and buckled. Bond length contractions parallel and perpendicular to the surface occur; the Pt top layer is rotated by a small angle (0.7°) with respect to the substrate. A second model that cannot be ruled out by the LEED analysis, but disagrees with ion-scattering data, involves shifted close-packed rows of top-layer atoms and requires domain structures in the case of Pt and Au. Charge-density-wave and missing-row models are ruled out by our structure analysis. A correlation is found between the occurrence of surface reconstructions on metals and a small ratio of their Debye temperature to their melting point. This correlation singles out mainly the 5d metals as having a propensity to surface reconstruction. The effects of adsorbates on the reconstructions are also discussed.