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Abstract | Full Text (PDF, 316KB)

Title: STUDIES OF CLEAN METAL SURFACE RELAXATION EXPERIMENT–THEORY DISCREPANCIES

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Abstract: A series of Low-Energy Electron Diffraction Intensity vs. Voltage (LEED I–V) measurements for Rh(001), W(110) and Ti(0001) have been undertaken in order to help resolve discrepancies between experiment and theory for the surface relaxations of certain transition metals. LEED measurements and analysis indicate the following results for the change of first (d_{12}) and second (d_{23}) interlayer spacings, relative to the bulk interlayer spacing d_0: for Rh(001), $\Delta d_{12}/d_0$=-1.4± 1.4% and $\Delta d_{23}/d_0$=-0.6± 1.4%; for W(110), $\Delta d_{12}/d_0$=-3.0± 1.3% and $\Delta d_{23}/d_0$=+0.2± 1.3%; and for Ti(0001), $\Delta d_{12}/d_0$=-4.9± 1.0% and $\Delta d_{23}/d_0$=+1.4± 1.0%. In each case, the new measurements help to resolve the experiment–theory surface relaxation discrepancies. In addition, two of these surfaces [W(110) and Ti(0001)] show substantial contractions in the first interlayer spacing, d_{12}. Large relaxations for close-packed surfaces lend support to the promotion–hybridization picture of surface relaxation put forth recently by P. J. Feibelman [P. J. Feibelman, *Phys. Rev.* **B53**, 13740 (1996).] In addition to making new experimental determinations of surface relaxations, a secondary goal of this work is to characterize sources of error associated with LEED I–V methodology that have traditionally not been fully appreciated.