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Structure of the SnO_2 (110)-(4×1) with LEED I(E)

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Tin dioxide (SnO2) is widely used as the active component of solid state gas sensors [1], and also has application in heterogeneous catalysis [2]. The basis for these applications is the reducibility of the oxide. The changes in conductivity of this n-type semiconductor resulting from surface processes are the basis for the material's gas-sensing characteristics. Because of this, it has long been a goal of fundamental research to characterize the structural, physical and chemical properties of SnO2 surfaces.

This work presents a quantitative low energy electron diffraction (LEED) analysis for the (4×1) reconstruction of SnO2 surface. A set of I(E) data for 15 inequivalent beams were collected with cumulative energy range of 1800 eV. The theoretical LEED intensities were fitted by using SATLEED program package [3]. The atomic coordinates for the Sn6O6 structure from a DFT calculation, scaled to the experimental lattice parameter of SnO2, were used as initial coordinates. The best fit structure, which differs from the DFT result by only a small (<0.1 Å) inward relaxation of the 6 Sn atoms, gives a Pendry reliability factor (RP) [4] of 0.16, indicating that the model describes the experimental data well.

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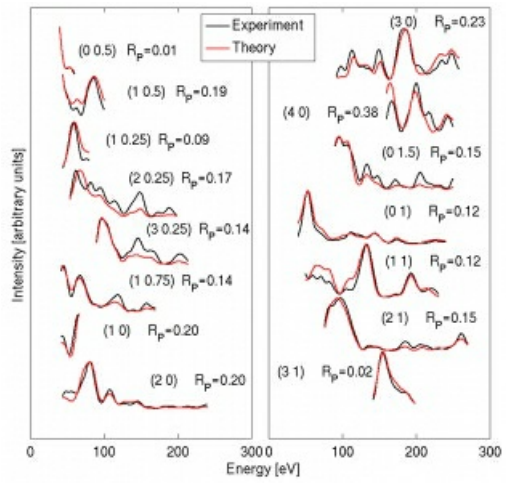

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