SURFACE STRESS DETERMINATION USING LOW-ENERGY ELECTRON DIFFRACTION

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The modified interactions on solid surfaces as compared to those in the bulk often result in surface stress. The surface atoms prefer to be closer together or further apart than the bulk lattice spacing, putting them under tensile or compressive stress, respectively [1].

Although the presence of surface stress is a well known phenomenon, its quantitative determination is still a challenge, both experimentally and theoretically. The most common experimental approach is based on measuring the bending of a thin sample upon adsorption of a foreign species on one side. This macroscopic effect is directly related to the change in the surface stress, but the method suffers from the averaging over the whole area. On the theoretical side, density-functional theory (DFT) calculations give reliable results for the bulk elastic parameters, while the studies of surface elasticity are complicated by the large supercells and demanding convergence criteria.

Our work shows that careful low-energy electron diffraction (LEED) measurements can give quantitative information on the surface stress [2]. The analysis is based on the lattice relaxations upon stress release at a boundary. Previously, a change in unit volume observed in small crystallites had been attributed to strain relaxation. In a similar fashion, we followed the changes in the average lattice constant in small *two-dimensional* oxygen islands on W(110), and combined the diffraction analysis with DFT calculations [2].

Oxygen adsorbed on a W(110) surface orders into a p(1×2) structure for coverages below 0.5 ML. At low coverages, the oxygen adatoms pack into islands, which grow in size with increasing coverage. At 0.5 ML, the whole surface is covered with the p(1×2)-ordered oxygen, whereas higher coverages result in structures with higher packing density.

Figure 1a displays the microspot-LEED pattern showing the two rotational p(1×2) domains (measured in a 2 micron diameter area with a single atomic step). The width of the diffraction spots gives the average island size (or domain size at higher coverage). We found that the half-order spot separations change systematically as the oxygen coverage is increased and the spots get sharper. This corresponds to a variation in the average distance between the oxygen atoms. The fractional changes in the spot separation have an inverse relation with the island size, as shown in Figure 1b. This inverse scaling is explained by a finite-length Frenkel-Kontorova chain, with the magnitude of the lattice relaxations proportional to the surface stress change across the island boundary [2]. Using calculated force constants, we obtained $\Delta\tau$ = -6.5 N/m along $[1\bar{1}0]$ as the stress difference between the oxygen covered and the clean tungsten surfaces.

For comparison, we performed DFT pseudopotential calculations using the PWSCF code. We utilized a thick symmetric slab to simulate the clean and oxygen covered tungsten surface. The structural parameters and the surface energy from our calculation showed good agreement with the data from the literature [2].

The calculated surface stress change between oxygen covered and clean W was found to be $\Delta\tau$ = -4.72 N/m, in fair agreement with the experiment despite the approximations in the experimental model. The level of this agreement is highlighted by a comparison

with the existing crystal-bending data [3], which lead to significantly lower values. We attribute the difference to the macroscopic nature of the crystal-bending measurement, which is avoided in our microspot diffraction data. Clearly the calculation does not take into account any surface defects, and a quantitative comparison is only possible with an experiment using a defect-free surface.

In addition to the surface stress values, the calculation gave further insight into our experimental observations. As seen in Figure 1c, the mismatch in the oxygen lattice along [001] scales with a higher power of the inverse island size. The calculations predict a very small stress change along the [001] direction, which is not sufficient to cause any significant lattice relaxation. However, stretching the calculation slab along [1$\bar{1}$0], a small stress is induced along [001]. This stress-strain coupling between orthogonal directions gives an explanation to the experimentally observed higher-order scaling along the [001] direction.

In conclusion, we show that, using low-energy electron diffraction, it is possible to extract quantitative information on surface stress. We expect our analysis to be of general use, beyond the specific O/W(110) adsorbate system studied here

References

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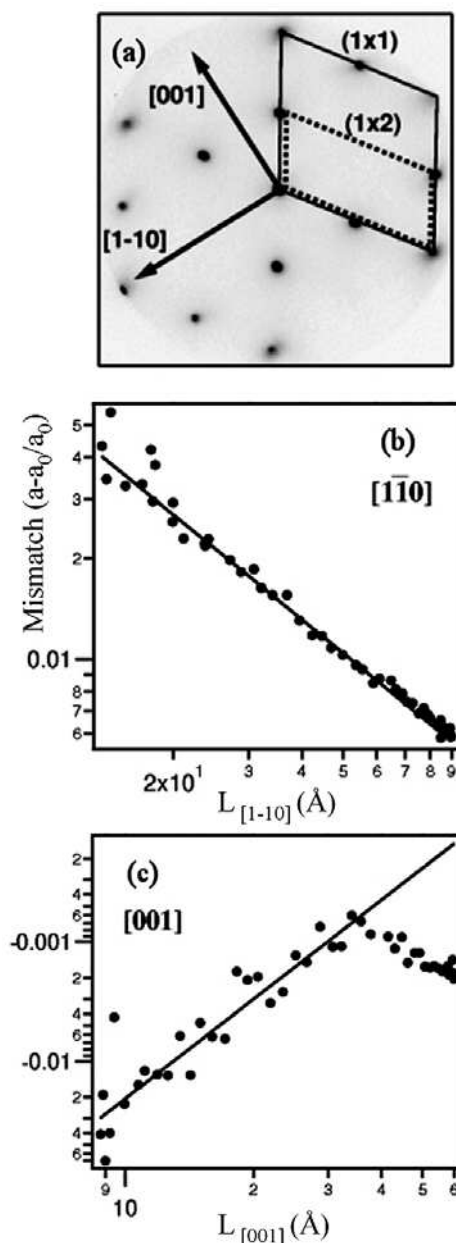[3] D. Sander, A. Enders, J. Kirschner, *Europhys. Lett.* **45**, 208 (1999).

Figure 1.
(a) LEED pattern of the p(1×2) oxygen covered surface.
(b) and (c) the evolution of the average oxygen lattice as a function of average island size along [1$\bar{1}$0] and [001], respectively.