SUBLATTICE IDENTIFICATION BY NON-CONTACT AFM ON THE (001) SURFACE OF A ROCKSALT-TYPE CRYSTAL

R. Hoffmann[1,2], L.N. Kantorovich[3], A. Baratoff[1], H.-J. Hug[1] and H.-J. Güntherodt[1]

1. Institute of Physics and National Center of Competence in Research on Nanoscale Science, University of Basel, Klingelbergstr. 82, 4056 Basel, Switzerland

2. Physics Institute, University of Karlsruhe, 76128 Karlsruhe, Germany

3. Dept. of Physics and Astronomy, King's College, London, WC2R2LS United Kingdom

E-mail: r.hoffmann@physik.uni-karlsruhe.de
§http://www-pi.physik.uni-karlsruhe.de

Dynamic force microscopy has proven able to achieve true atomic resolution on the surface of different materials in UHV, insulators in particular [1]. Owing to imperfect knowledge about the structure and composition at the apex of the imaging tip, it is, however, difficult to assign observed features to specific atomic sites. On ionic crystals, a common approach is to compare experimental images with simulations relying on plausible models of the tip apex and fitted interionic potentials. Thus, on the CaF_2(111) surface, F^- ions at inequivalent sites could be distinguished [2]. On the (001) cleavage plane of crystals with the rocksalt structure, however, one kind of ion is imaged as a maximum, and the other kind as a minimum. Owing to the high symmetry, it was deemed impossible to determine which sublattice is imaged because the sign of the electrostatic potential near the tip apex is not known a priori.

By comparing force-distance curves extracted from cantilever frequency shifts measured above specific sites with calculated forces, we show that recognition is in fact possible. First, as indicated by simulations, the short-range forces above the saddle point centred between two adjacent maxima and minima in an image differ for a positively or negatively terminated tip. Next, site-independent long-range forces can be eliminated by considering differences between forces at particular sites. As first demonstrated on the Si(111)7x7 surface [3], the required accuracy can be obtained using a PLL-controlled frequency detection and cantilever excitation scheme and an essentially drift-free low-temperature instrument.

Results are illustrated for the KBr(001) surface, using the same model as in ref. 2, but assuming a $(KBr)_{32}$ cubic cluster at the tip apex. Indeed, contrast changes suggest that material was picked up from the sample while scanning to locate a flat area. A comparison of the difference between forces obtained above the maximum and the minimum agrees better with the corresponding difference calculated for the tip with K^+ at the apex once the experimental distance scale offset is adjusted to achieve best agreement beyond 0.5 nm. The corresponding differences between forces above the saddle point and the maximum then match only for the positively terminated tip. Because the strongest attraction occurs above sample ions with the opposite sign, maxima in images at constant negative frequency can be assigned to the Br^- sublattice [4].

This proceure is expected to remain valid for (001) surfaces of other crystals or ultrathin films with the same structure. It might help determine the relative location and charge of characteristic surface point defects on such surfaces, e.g. catalytically active sites on oxides of divalent metals.

References:

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Figures:

Figure 1: Topographic image recorded at a constant frequency shift of -19.5 Hz on the KBr (001) surface.

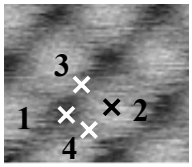

Figure 2: Comparison of the calculated and the measured force differences for the force above sites (3) and (2) identified in figure 1.