Functional Materials

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Atomic resolution interface study of VN and Cu films on MgO using spherical-aberration corrected TEM

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Interfaces strongly influence the functional and mechanical properties of materials. Recent advancements in TEM instrumentation permit to image the structure of material defects at atomic resolution and with elemental sensitivity by correcting the spherical aberration of the objective lens. In the present talk this benefit will be illustrated using two different material systems. The first system is a ceramic-ceramic structure consisting of VN on MgO, while the second is Cu on MgO. While for VN on MgO the misfit is quite low with 0.7% Cu on MgO possesses a large mismatch of 14.1%. For both systems the interface structure is analyzed with respect to its atomic structure using a 200 kV field emission TEM/STEM (JEOL 2100F) equipped with an image-side C_S-corrector.

Determination of the atomic positions with picometer precision reveals subtle periodic oscillations in the VN (Fig. 1) and Cu (Fig. 2) adjacent to the interface, while this is not observed for MgO. The analysis of the atomic displacements for VN on MgO reveals that the interplanar spacings oscillate adjacent to the interface in a similar way for both experimental measurements and DFT calculations [1]. The interfacial chemistry derived from ELNES with subnanometer spatial resolution revealed a V- and O-enriched interface where V-O bonds are likely to be formed at the interface, resulting in a slightly reduced V valence state.

For Cu on MgO the variations of the interplanar spacing adjacent to the interface show a damped oscillation similarly as for VN on MgO. Again, at the MgO side the oscillations are not pronounced as compared to the Cu side. The experimental measurement shows the oscillations down to around 13 layers. This phenomenon, we believe, is the Friedel oscillation occurring at the interfaces, which is similar to the Friedel oscillation present at the metal surface as observed in literature by scanning tunneling microscopy. The origin for the oscillatory interplanar spacing, i.e. contractions and expansions in lattice plane spacing, is most likely attributed to the repulsive or attractive atomic forces between the layers induced by electronic charge redistributions.

The possible impact of the interface structures observed by TEM on the material properties is briefly discussed.

1. Z. Zhang, B. Rashkova, G. Dehm, P. Lazar, J. Redinger, R. Podloucky, *Unveiling the atomic and electronic structure of the VN/MgO interface*, Phys. Rev. B 82, 060103(R), 2010 1-4.

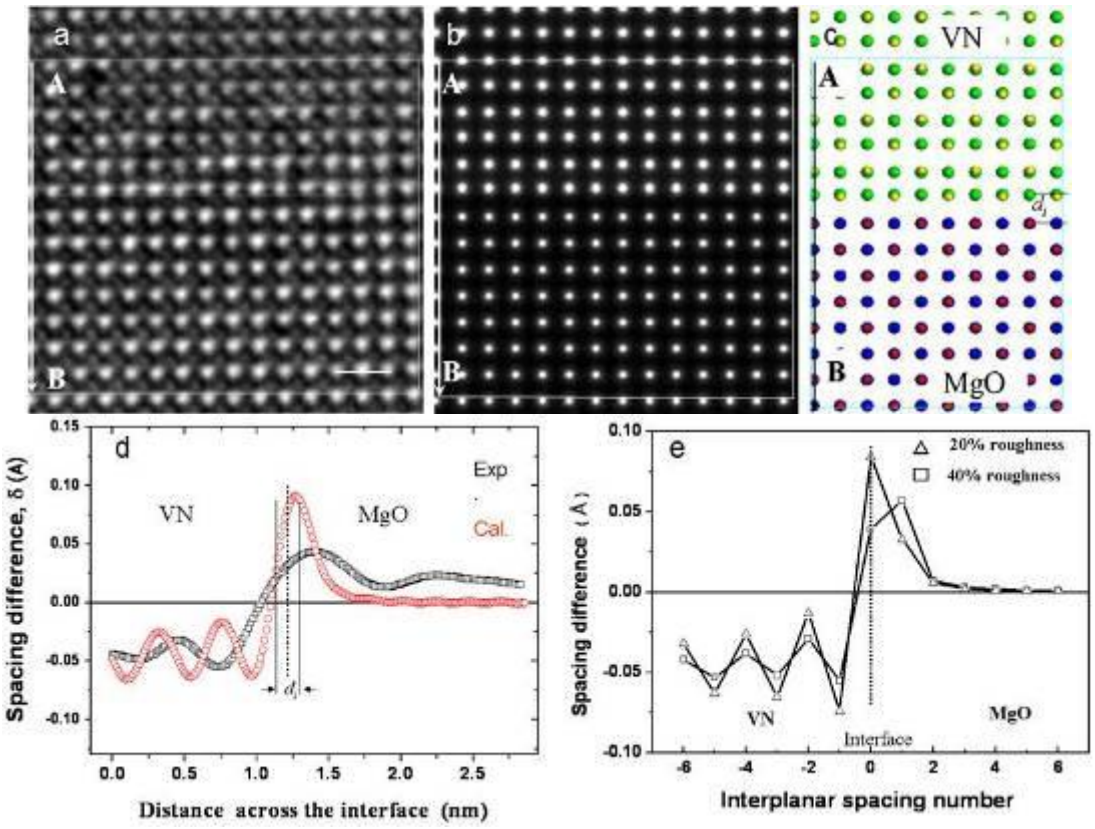

Figure 1. (a) A HRTEM image of the VN/MgO interface recorded along [100] (thickness: ~ 3.3 nm). A simulated potential image is shown in (b) based on an atomic model (c) obtained from ab-initio calculation. The spacing difference (d) obtained by averaging over a rectangular area of around 3.0 nm from A to B in (a), (b) is plotted as a function of distance covering 13 spacing of d_{002}, where the red and black curves denote the calculated (no roughness) and experimental results, respectively. The interfacial spacing d_i is indicated. Panel (e) shows the effects of an assumed mono atomic step roughness (20%, 40% roughness) Images and diagrams from [1].

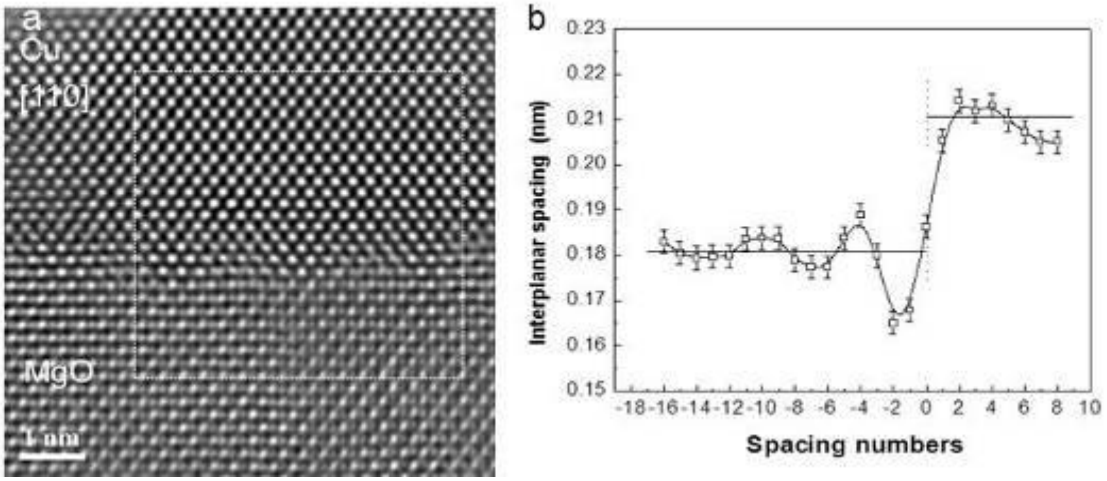

Figure 2. (a) HRTEM image of the Cu-MgO interface with a cube-on-cube epitaxial relationship, recorded along the [110] direction using a small negative C_S in which the individual O, Mg and Cu atomic columns are clearly imaged as bright dots (thickness: 2.0 - 3.0 nm). Paired dislocation components projected from the <100> misfit direction network are visible, and separated by coherent regions giving a little brighter contrast. (b) The (d_{002}) interplanar spacing is plotted as a function of interplanar spacing numbers across the interface. The thin lines denote the bulk Cu d_{002} and Mg d_{002} spacing, respectively.