

Atomic and Electronic Structure of Polar Fe₂O₃/MgO Interface

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To address the role of polarity on the growth and stability of heterointerfaces, we present an integrated experimental and *ab initio* investigation of the structural, electronic and magnetic properties of the layer-by-layer growth of Fe₂O₃(0001) thin films on polar MgO(111) substrate [1].

Hematite films were grown on hydrogen terminated unreconstructed MgO(111) polar surfaces by oxygen plasma assisted molecular beam epitaxy. Cross sectional samples were made for HRTEM studies by conventional mechanical polishing and argon ion milling methods before investigations with a JOEL 2200 aberration corrected transmission electron microscope using 200 keV electrons. Spin-polarized DFT calculations were done in a slab geometry using the full-potential linearized augmented plane wave (FLAPW) method as implemented in *flair*.

The heterointerface is atomically abrupt with Mg₃|O₃|Fe₂...oxide-like stacking for film thicknesses between ~ 1.5 -6.0 Å. The interface is found to be stabilized by drastic structural relaxations and its properties vary as a function of the hematite film thickness. Fig. 1(a) shows the initial and final atomic structure of a 3 Fe-bilayers film on MgO. The structural relaxations consist of interpenetration, separation, and merger of Fe and oxygen planes, as seen in Fig. 1(b), giving rise to a barrierless expulsion of oxygen and formation of an Fe₂|FeO₃ layer structure not seen in hematite. Atomic rearrangements are accompanied by polarization of electronic charges that screen the dipole field of the polar system and lead to (half-)metallic states throughout the film and to a variety of metastable magnetic configurations.

A reconstructed HRTEM phase image from a true focal series and an intensity profile across the interface from a single row of atoms is shown in Fig. 2. The ABC stacking in MgO is clearly resolved and proceeds all the way to the interface. The first three layers at the interface display a distinctly different structure than the hematite layers away from the interface in support of the theoretical predictions.

References

- [1] K. Pande, M. Gajdardziska-Josifovska, and M.Weinert. *Phys. Rev. B (submitted)*, 2009.
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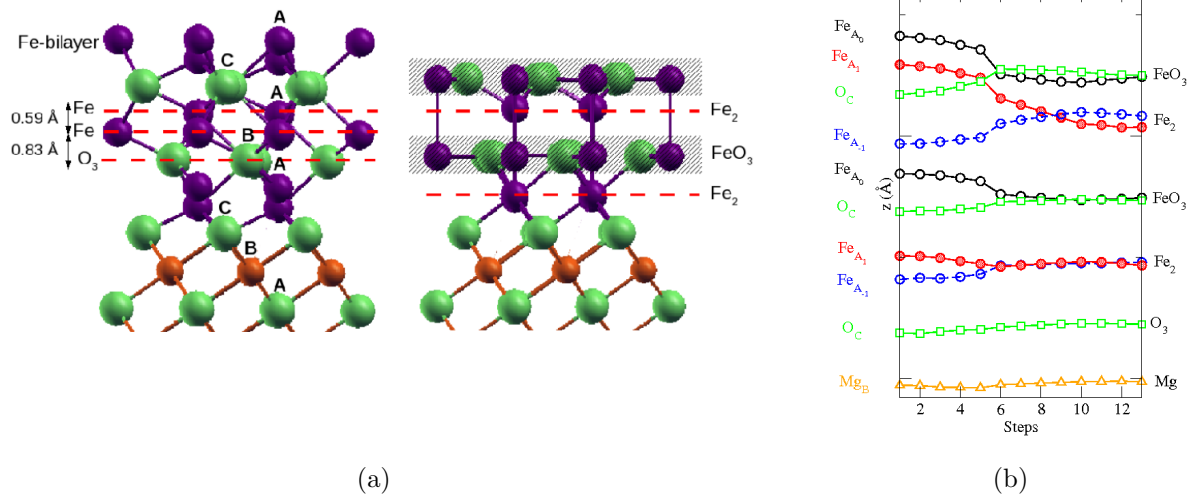


Figure 1: (a) Side view of unrelaxed and relaxed structures and (b) atomic positions as a function of relaxation steps for a 3 Fe-bilayers film.

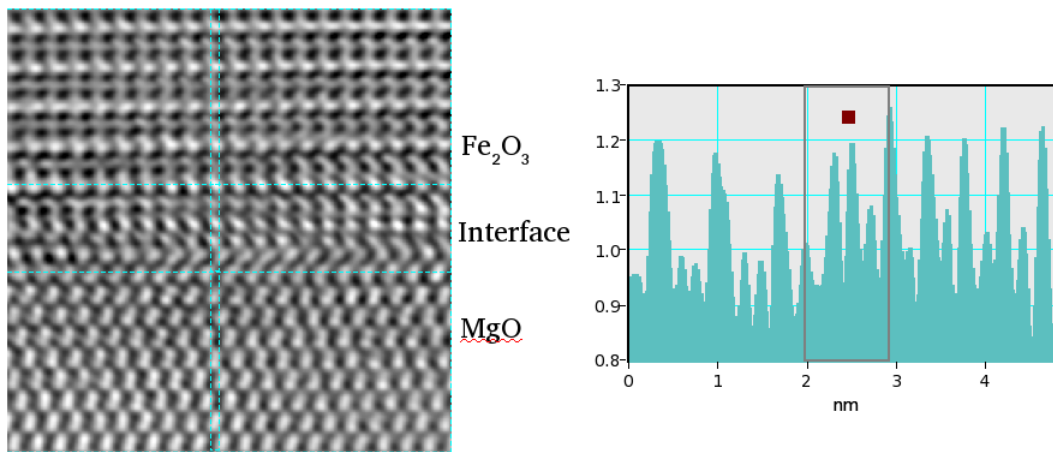


Figure 2: Intensity profile across the interface•