

Structure Determination of Fe₃O₄(111)/MgO(111) Polar Oxide Interface

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Polar oxide surfaces and interfaces are current frontier issues in surface science. The structure of polar oxide surfaces appears to be determined by the need to cancel the net electric dipole moment perpendicular to the surface, and hence produce finite surface energy. Various mechanisms such as: surface reconstruction, faceting, metalization, relaxation and adsorption have been proposed as a way to stabilize the polar oxide surfaces [1]. Both MgO (111) and Fe₃O₄ (111) polar surfaces have been studied in this context, and we recently initiated the first study of their interface discovering stabilization by formation of metallic Fe nanocrystals [2]. In this work we attempt to determine the atomic structure of the Fe₃O₄(111)/MgO(111) polar oxide interface using high-resolution transmission electron microscopy (HRTEM).

Magnetite films were grown by oxygen plasma-assisted molecular beam epitaxy on single crystals of MgO(111) with 1×1 surface structure. Standard polishing-dimpling-ion milling methods were used to prepare cross-sectional samples in <110> and <211> zones. A Hitachi H-9000 NAR microscope, operated at 300 keV and equipped with a Gatan slow scan CCD camera, was used to record digital through-focal HRTEM images. Through focal and thickness HRTEM maps were calculated using the EMS program package [3].

The experimental images rule out interface faceting as a possible stabilization mechanism, and indicate that the Fe₃O₄(111) film has preferred stacking, implying unique interface structure (Fig. 1). Comparison between experimental and calculated images in both [1-10] and [11-2] zones were performed for four model interfaces with different polarity. The best fit to the experiment is the interface determined by a monolayer of Fe in octahedral (Fe_B) position (Fig 2a) with the following stacking sequence: 4Mg/4O/3Fe_B/4O/Fe_A /Fe_B /Fe_A/4O. Models initiating with a full (Fig. 2b) iron three layer (Fe_A /Fe_B /Fe_A), or its two truncated variants (not shown here), where Fe in tetrahedral position is denoted as Fe_A, are lesser fit to experiment (Fig. 3).

In summary, this structure determination favors the interface model that starts with monolayer of Fe in octahedral position. Although interface models with truncated Fe three layer bear less electric dipole moment per unit cell, they do not match the experimental data, leaving the formation of Fe nano-inclusions as a main stabilization mechanism for the Fe₃O₄(111)/MgO(111) polar oxide interface [4].

[1] M.Gajdardziska-Josifovska et al., *J.Elec.Micr.* **51** (2002)

[2] V.K. Lazarov, S.A Chambers and M.Gajdardziska-Josifovska, *Phys. Rev. Lett.* (submitted)

[3] P.Stadelmann, *Ultramicroscopy* **21**,(1987)131.

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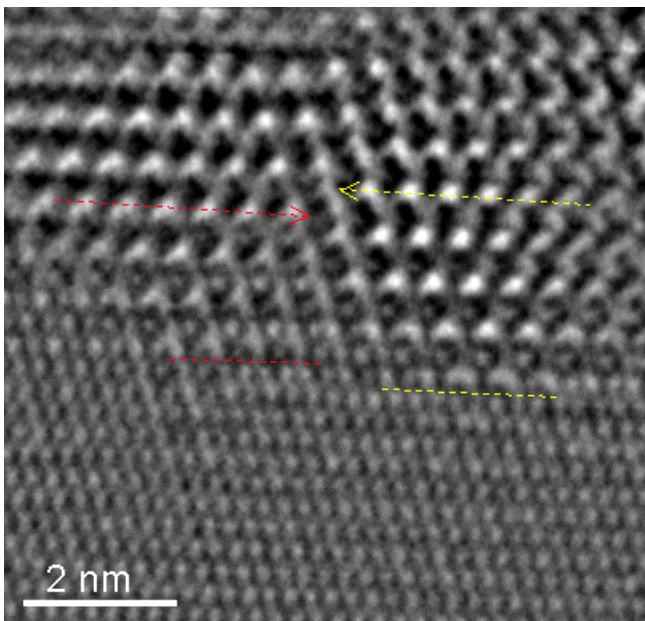


Fig 1. HRTEM in [1-10] zone showing that growth of $\text{Fe}_3\text{O}_4(111)$ on different $\text{MgO}(111)$ terraces initiates with same stacking. Grain boundary occurs for odd terrace step.

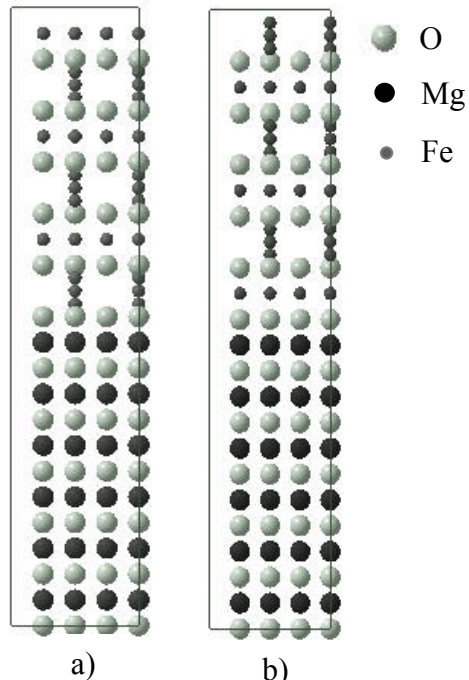
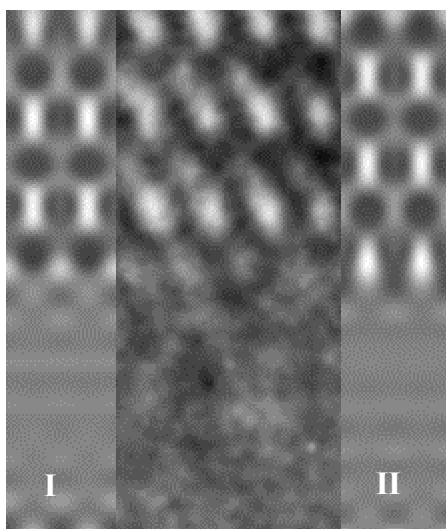
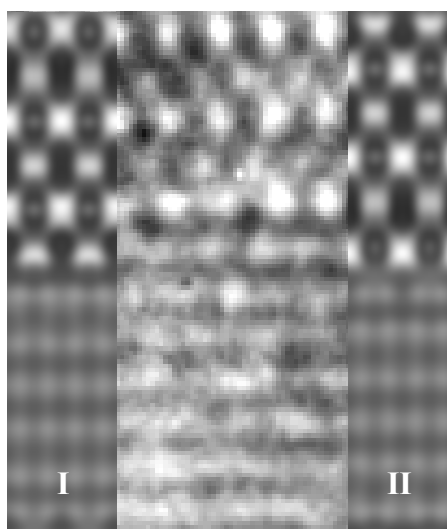


Fig 2. a) Model interface I initiating with monolayer of Fe_B . b) Model interface II initiating with three layer of $\text{Fe}_A/\text{Fe}_B/\text{Fe}_A$. Both models are shown in [11-2] projection.



a)



b)

Fig 3. Two members from through-focal series of HRTEM image matching in [11-2] zone at thickness of 6 nm and under-focus of 25 nm (a) and 65 nm (b). Interface I is better match to the experiment.