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# High Resolution Electron Microscopy Studies of Polar Oxide Interfaces

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The instability of polar surfaces is closely related to that of polar interfaces, resulting from the apparent presence of an electric dipole moment in the repeat unit parallel to the surface/interface. Studies of polar semiconductor interfaces, based on classical electrostatic models, exclude the existence of atomically abrupt polar semiconductor interfaces to avoid the huge dipole fields that would otherwise arise at the interface, and consequently produce interface charge accumulation. In this classical model, atomically abrupt polar oxide interfaces are even less likely, since ionicity in oxides is more pronounced. Thus the question of polar oxide interface stability remains open for both experiment and theory. We are recently undertaking extensive High-Resolution Transmission Electron Microscopy (HRTEM) experiments and simulations, backed by Density Functional Theory (DFT), to study surface and interface polarity effects on the atomic and electronic structure of $Fe_3O_4$/MgO(111) [1,2] and GaN/MgO(111) [3] model polar interface systems. These results, like other interface structure determinations, have been enabled by John Maxwell Cowley's lifetime contributions to the development of HREM theory and experiment.

Magnetite films in their polar (111) orientation were grown by plasma assisted molecular beam epitaxy on the MgO(111) polar surface. In difference to $Fe_3O_4$ films grown on lattice matched metal substrates and on the neutral MgO(100) surfaces, we found phase separation in the polar case, with formation of Fe nanocrystals at the interface and within the polar magnetite film [2]. HRTEM imaging and DFT calculation showed that atomically abrupt interface structure can exist between the MgO(111)-substrate and $Fe_3O_4$ (111) film in regions separated by Fe nanocrystals. Fig. 1 shows two such interface regions, illustrating the occurrence of inverse domain grain boundaries where the film grows on terraces separated by odd number of steps (Fig. 1a). These defects are absent on even stepped terraces (Fig. 1b), a sign of preferred $Fe_3O_4$(111) film stacking. Comparison of through-focus/through-thickness experimental HRTEM images with calculated images (not shown here for lack of space) finds metal-oxygen-metal (i.e. Mg-O-Fe) interface bonding with octahedral (B) coordination of the first Fe monolayer, rather than the ABA tetra-octa-tetrahedral stacking or its BA and A models created by Fe vacancies. While all models produce metal induced gap states for the interface oxygen layer, the winning model provides lowest total energy with an effective screening of the MgO(111) substrate surface polarity. The data and calculations exclude mixing of Mg and Fe across the interface.

Our most recent ongoing project has found that the MgO(111) surface polarity can be used for selected growth of cubic zinc-blende (111), or hexagonal wurtzite (0001), GaN films by controlling the nature of the first interface layer [3]. The cubic stacking is enabled by nitrogen induced polar surface stabilization, predicted to yield MgO(111)-(1×1)-ON metallic surface structure. HRTEM (e.g. Fig. 2) and DFT studies indicate that the atomically abrupt semiconducting GaN(111)/MgO(111) interface is determined by Mg-O-N-Ga stacking, with each N atom bonded to O at top site, and with Ga polarity of the film. This specific atomic arrangement at the interface allows cubic stacking to more effectively screen the substrate and film electric dipole moment then the hexagonal stacking, stabilizing the zinc-blende phase.

In summary, substrate polarity cancellation appears to be a driving force that determines the atomic structure of the studied polar oxide/oxide and oxide/nitride interfaces. Charge redistribution at the interface effectively screens the interface dipole moment, enabling existence of chemically abrupt interfaces [4].

[1] V. K. Lazarov, Ph.D. dissertation, University of Wisconsin Milwaukee (2004).
[2] V. K. Lazarov, S. Chambers and M. Gardardziska-Josifovska, *Phys. Rev. Lett.* **90** (2003) 216108.
[3] V. K. Lazarov et al., *Phys. Rev. Lett.* (2005) in review.
[4] Funding by NSF and Research Corporation, and collaborations with S.A.Chambers, L. Li and S. H Cheung (MBE) and M. Weinert (DFT) are acknowledged.

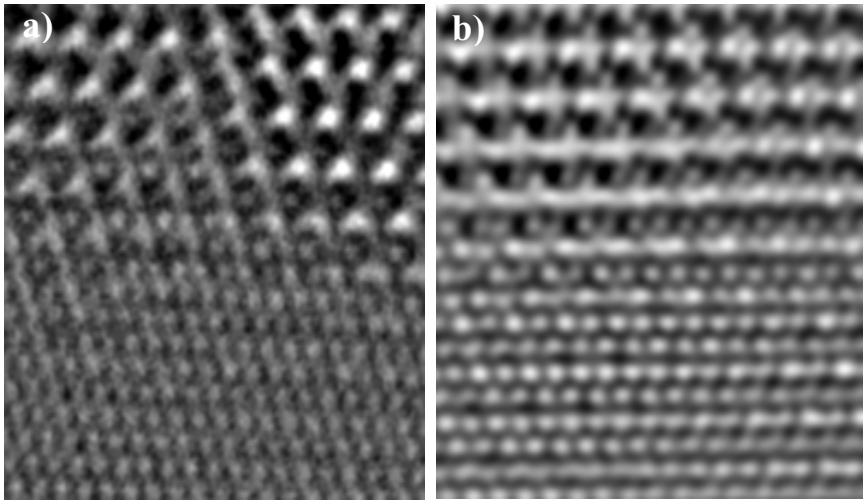


Fig. 1. HRTEM of $Fe_3O_4$(111)/MgO(111) interface from regions with steps on the MgO surface: a) For odd step height (i.e. one Mg-O bilayer), lattice misalignment is observed in magnetite film indicative of grain boundary; b) No grain boundaries are present when step height is even (i.e. two Mg-O bilayers).

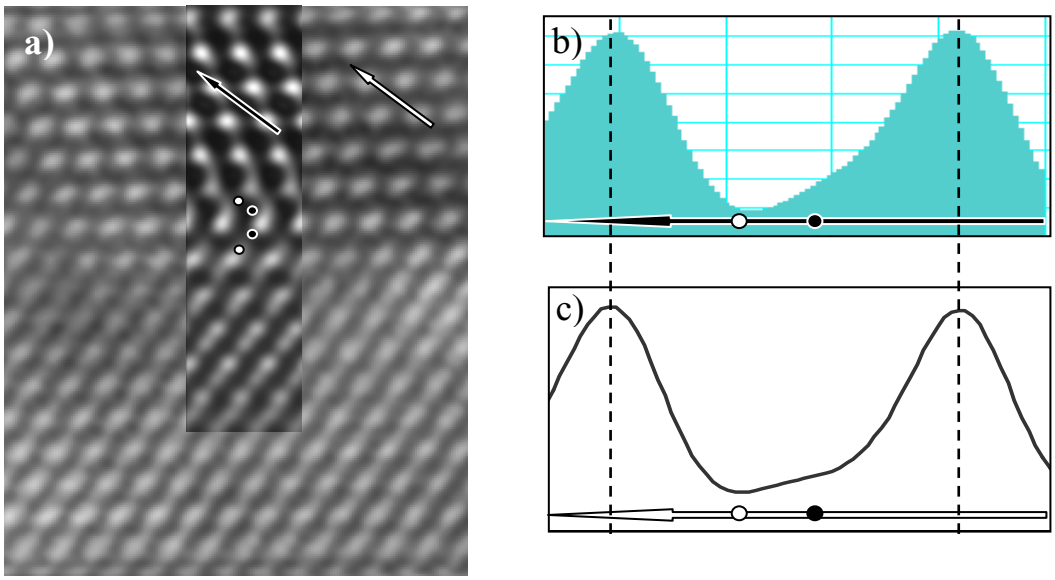


Fig.2 a) Experimental HRTEM image of c-GaN(111)/MgO(111) interface with inset showing best fit simulated N-top model with Mg-O-N-Ga stacking. b) calculated intensity profile from bulk c-GaN along dumbbell direction showing asymmetry towards Ga; c) averaged experimental intensity profile along 25 dumbbells (in direction indicated with arrow on image a) indicating Ga film polarity.

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