MS-12-P-3272 Atomic and electronic structure of Fe₃O₄ oxides heterostructures

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Magnetite (Fe₃O₄) has recently attracted a lot of attention for future spintronic applications due to its 100% spin polarization at the Fermi level [1]. Incorporating magnetite thin films as an electrode in heterostructures such as spin valves, magnetic tunnelling junctions and other device structures requires growth with atomic control of Fe₃O₄ thin film interfaces with oxide tunnel barriers and semiconductor layers. Therefore understanding the atomic and electronic structure of Fe₃O₄ interfaces is crucial for any future development of devices based on halfmetallic Fe₃O₄.

In this work we study two interfaces of Fe₃O₄; with MgAl₂O₄ as a model tunnel barrier and doped SrTiO₃(111) as a semiconductor layer important for spin injection and diffusion. Fe₃O₄ thin films were grown by MBE and PLD and post annealed ex-situ in a CO/CO₂ atmosphere in order to improve their stoichiometry and structural ordering. Structural analysis was performed by TEM/STEM and EELS using aberration corrected JEOL 2200FS, Nion Ultrastem 100, and JEOL ARM 005. Electronic calculations have been performed with DFT using full and pseudo potential plane wave codes.

(Fig. 1) shows the interface region of Fe₃O₄(111)/MgAl₂O₄(111) in a cross-sectional [1-10] viewing direction. The MgAl₂O₄ substrate and Fe₃O₄ layers share the same spinel structure. By following the stacking across the interface we show the FCC O sublattice common to both structures is uninterrupted across the interface. HAADF modelling indicates the sharp interface is defined by the stacking sequence: (…/4O/Mg-Al-Mg/4O/3Fe₈/4O/…), where Mg is in a tetrahedral site while Fe₈ and Al are in octahedral sites. The DFT calculations confirm this interface is the lowest energy. Similarly to Fe₃O₄/MgAl₂O₄ the Fe₃O₄/SrTiO₃(111) interface is atomically sharp as shown in Fig. 2. defined by (…SrO₃/Ti/Fe₈/4O/3Fe₈…). The clear presence of misfit dislocations in both interfaces is seen. By using GPA analysis we evaluate the strain around the dislocations cores. Finally we performed electronic spin density calculations on the best experimentally matched models as well as other plausible models, and we show that sharp interfaces with bulk like stacking sequence maintain spin polarization.


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Fig. 1: HAADF STEM image of the interfacial region of Fe$_3$O$_4$/MgAl$_2$O$_4$(111) in the cross-sectional [1-10] viewing direction.

Fig. 2: HAADF STEM image of the interfacial region of Fe$_3$O$_4$/SrTiO$_3$(111) in the cross-sectional [1-10] viewing direction.