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Atomic study of $Fe_3O_4/SrTiO_3$ Interface

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Complex oxide heterostructures are of interest for developing new functional materials due to their rich physical properties [1]. Many oxides are insulators, but also wide band gap semiconductors, superconductor, ionic conductors, ferrimagnetic and antiferromagnetic materials. Hence oxide heterostructures provide a broad platform for devices with multifunctional properties. The functionality of those devices strongly depends on the atomic scale structural and electronic discontinuities across the multilayer heterostructural interfaces; therefore the need for atomic scale understanding of their properties. In this work we focus on spinel-perovskite heterostructures that have potential for the development of multiferroic devices by using $Fe_3O_4/StTiO_3$ as a model system [2,3]. This heterostructure is of importance for spintronic applications but also it represents a class of heterostructure that can host ferrimagnetic and ferroelectric properties which can be coupled through suitable interface engineering.

The Fe_3O_4 films were grown on $SrTiO_3$ (STO) substrate by pulse laser deposition techniques. A post-annealing has been undertaken in order to improve films structure and stoichiometry [4]. The overall structure of the films was determined by X-Ray diffractometry. Atomic and electronic study of the Fe_3O_4/ $StTiO_3$ interface was performed using scanning transmission electron microscopy and electron energy loss spectroscopy with a JEOL 2200 FS TEM/STEM and a Neon Ultrastem 100. First principle calculations were also performed in order to determine the spin/electronic properties in the near interface region of the Fe_3O_4/ STO from the several model interfaces.

Fig. 1 shows that the Fe_3O_4 film has a uniform thickness and single crystal structure. The epitaxial relation between the film and substrate is the standard cube on cube as following: $Fe_3O_4(111)||STO(111)$ and Fe3O4(11-2)||STO(11-2). The annealing of the film has improved the structural ordering as indicated in Fig.2. Moreover the annealing significantly reduces the number of antiphase domain boundaries in the film (not shown here). The atomically resolved electron energy loss spectroscopy shows that the film/substrate interface is atomically sharp, and that no atomic mixing is present. The lattice mismatch between the film and substrate introduces an interfacial strain which is relieved by formation of interfacial periodic misfit dislocations. The region between the dislocations has well defined atomic structure (Fig.2). The most favourable model that fits the best the STEM-HAADF data is determined by ../Ti/O/Fe_B/.. atomic planes, where Fe_B represent the Fe octahedral planes in magnetite. The first principle calculations has found that atomic mixing at the interface is not favourable. In addition the calculations show that electronic structure of this, polar in nature, interface is very sensitive to the atomic structure; with the band offsets and Fermi level position different and uniquely determinant for the all abrupt interface models considered.

References

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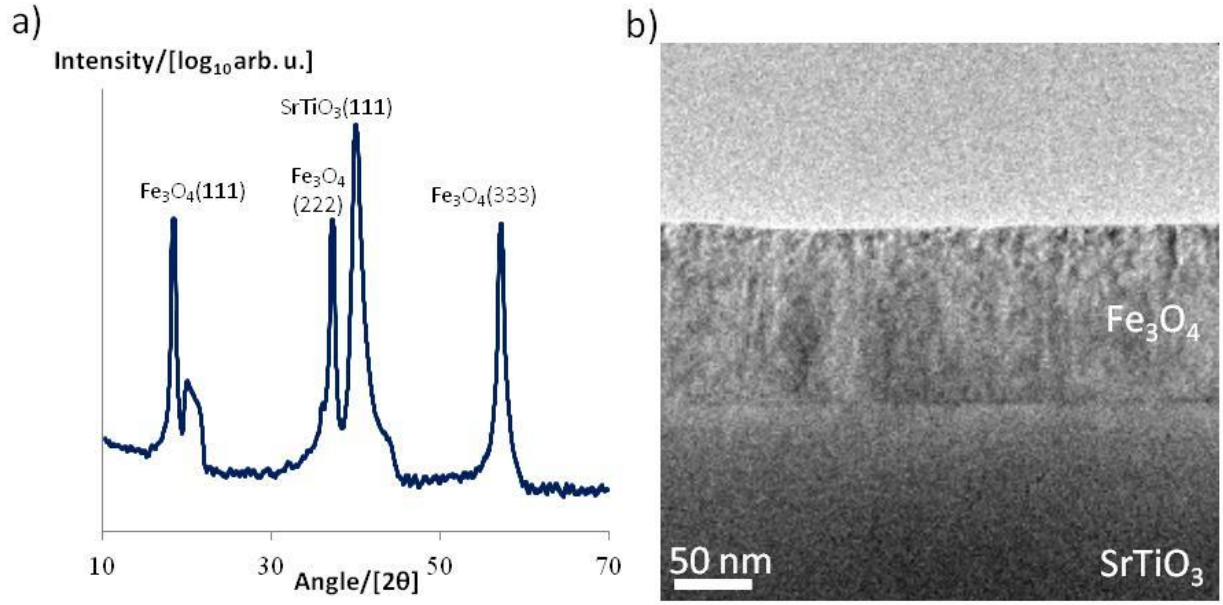

Fig. **1**: $Fe_3O_4/SrTiO_3(111)$ interface. **a)** θ-2θ x-ray diffraction shows single phase Fe_3O_4 film with parallel (111) planes shared between the film and the substrate in the growth direction. **b)** Low magnification image of the $Fe_3O_4/SrTiO_3$.

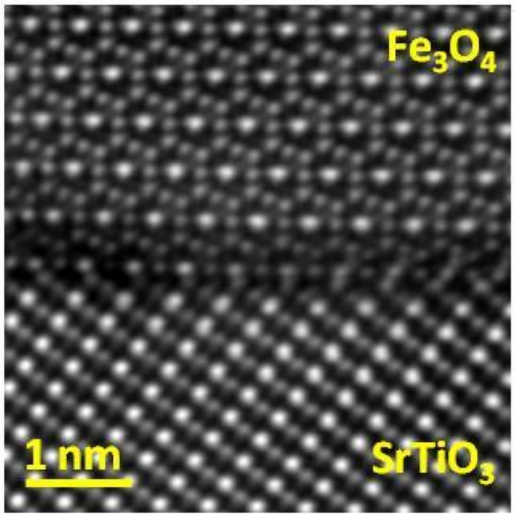

Fig.**2**: Atomically resolved HAADF-STEM image of the $Fe_3O_4/SrTiO_3$ interface in the [1-10] zone axis.