Synchrotron X-ray Analysis of the MBE-Grown Fe_3O_4 Epilayer on MgO (001)

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Making use of high-resolution X-ray diffraction, we characterized an MBE-grown Fe_3O_4 epilayer on MgO (001) substrate and determined the thickness to be 793 Å with the lattice constants $a = b = 8.413 \pm 0.013$ Å, $c = 8.366 \pm 0.001$ Å. Compared to the MgO lattice constant, a_S= 4.213 Å, this Fe_3O_4 layer was coherently strained on the substrate. Regarding the electronic structure, the DANES spectrum of Fe_3O_4 (115) revealed more apparent features of the resonant excitation through the electronic quadrupole transition than the case of (004) diffraction, while RXS spectra of the forbidden (002) reflection revealed similar resonance features from room temperature down to 90 K. We conclude that (*hhl*) diffraction and the associated forbidden reflections with $h \neq 0$ would be a better choice to explore the origin of the Verwey transition in magnetite.

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I. INTRODUCTION

Magnetite, Fe_3O_4, is one of the most famous magnetic minerals due to its ferrimagnetic property, metal-to-insulator transition, and potentially half-metallic applications to spintronics. From an ionic picture, because the super exchange interaction mediates a ferrimagnetic order when the temperature of magnetite is below T_C (858 K), the anions O^{2-} and cations Fe^{3+} and Fe^{2+} form an inverse spinel structure, $[Fe_A^{3+}O][Fe_B^{3+}Fe_B^{2+}O_3]$. The Fe^{3+} ion of the sublattice A is bound with four nearest-neighbor oxygen ions so as to form a tetrahedron, while the other Fe^{3+} and Fe^{2+} ions are mixed on the sublattice B and each B-site cation is bound with six oxygen ions to form an octahedron. At room temperature, the lattice structure of bulk magnetite crystal is cubic and belongs to the $F_{d\bar{3}m}$ space group, with the lattice constant a_B= 8.397 Å.

Back in early 1941, Verwey [1] discovered an unusual first-order phase transition of the magnetite crystal around the temperature of T_V (~122 K). When cooled from above, the electrical resistance of magnetite at T_V increased by nearly two orders of magnitude. Because the origin of the Verwey transition is still debated, recent research efforts have been focused on studying whether the electron transport property is localized due to charge separation of B-site cations or not [2, 3]. In spite of experimental measurements achieving very high accuracy nowadays, this long-time argument still remains a puzzle.

Resonant X-ray scattering (RXS) is a powerful synchrotron X-ray technique for singling out a particular ordered structure among the valence electrons [4]. Regarding the

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