Link between local iron coordination, Fe 2p XPS core level line shape, and Mg segregation into thin magnetite films grown on MgO(001)

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A well-ordered Fe(001) ultra-thin film epitaxially grown on MgO(001) has been oxidized by post deposition annealing in oxygen atmosphere. LEED patterns indicate the formation of magnetite (Fe_3O_4) after one hour of oxygen exposure. The LEED pattern remains stable despite annealing the sample for further four hours. In contrast X-ray Photoelectron Spectroscopy (XPS) of the Fe 2p core levels suggests the formation of an iron oxide comprising mostly of merely trivalent iron. This discrepancy is analyzed and discussed employing charge transfer multiplet calculations for the Fe 2p XPS spectra. We find that Mg ion segregation from the substrate into the magnetite thin film replacing octahedrally coordinated Fe^{2+} ions and the excess occupation of octahedral sites which are unoccupied in the ideal inverse spinel structure are driving forces for the altered shape of the Fe 2p XPS spectra. Different potential models which might explain the nature of the Mg ion segregation into the magnetite films are discussed.