

# Structural Model for the X-ray Resonant Scattering: Half-Doped Manganites and Magnetite

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We review our recent studies on the occurrence of atomic charge localization in magnetite and half-doped manganites. X-ray resonant scattering experiments at the Fe K-edge of magnetite and at the Mn K-edge in  $\text{Nd}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$  show the lack of atomic charge localization on the transition-metal atom. The evolution of the intensity of the (002) and (006) forbidden reflections in magnetite across the Verwey transition with the incoming x-ray photon energy, the dependence on the azimuthal angle and the polarization of the scattering process show that the atomic anomalous scattering factors for the octahedral Fe ions are identical to each other, i.e. all of them show the same electronic state [1,2]. On the other hand, the dependence of the x-ray resonant scattering intensity of the satellite reflections (3 0 0), (0 3 0) and the forbidden reflection (0 5/2 0) on the photon energy, the azimuthal angle and the x-ray polarisation in the low temperature phase of  $\text{Nd}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$  has been also analysed using a semi-empirical structural model. Contrary to previous claims of atomic charge and orbital ordering (COO), we show that the dipole resonant superlattice reflections can be explained by the presence of two types of Mn sites with different local structure. One of the Mn sites is surrounded by a tetragonal-distorted octahedron of oxygen atoms whereas the other site has a symmetric octahedral environment. The model establishes the lack of integer ionic ordering and the observed resonances are mainly explained as arising from the geometrical local anisotropy. Intermediate valences according to a fractional charge segregation  $\text{Mn}^{3.42}\text{-Mn}^{3.58}$  were deduced [3]. Both, the Verwey transition in magnetite and the COO transition in manganites, can be well described as structural phase transitions where a phonon mode condenses giving rise to a new periodicity mainly associated to the oxygen atoms.

## References

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