

Electron-Phonon Coupling in the Presence of Charge-Orbital Ordering in Magnetite Fe₃O₄

At the Verwey transition temperature $T_V = 122$ K the resistivity of Fe₃O₄ jumps by two orders of magnitude from a metallic to an insulating state accompanied by a structural symmetry change. Resonant x-ray scattering has shown that the charge and orbital orderings set in at temperatures above T_V [1]. This suggests that the electronic energy is released into a lattice relaxation on lowering the temperature across T_V . The transition is of first order with no single symmetry element connecting the high temperature and low temperature phases, while combination of X₃ and Δ_5 can parameterize the transition [2].

We have measured the phonon dispersion of low-lying branches connecting to X₃ and X₄ along the Δ and Σ directions at various temperatures above T_V by inelastic x-ray scattering. The Δ_5 -X₄ branch has anomalously large phonon widths at room temperature that broaden further on lowering the temperature to T_V . The X₃ phonon shows the normal behaviour of sharpening up with lowering the temperature.

Calculations of the lattice dynamics using local density approximation (LDA) and its extension to on-site electron-electron correlations (LDA+U) using $U = 4$ eV show strong anharmonicity in the X₄ branch while the X₃ branch is only mildly anharmonic. The anharmonicity disappears for $U = 0$. We thus conclude that the electron-phonon coupling is strongly influenced by the electron-electron correlations. This effect of correlations explains the large difference in width in the two branches we observed and may account for the electron-lattice coupling manifest in the structural phase transition. This result demonstrates that the Verwey transition is a cooperative phenomenon which involves strongly correlated electrons coupled to lattice degrees of freedom.

[1] J. E. Lorenzo et al. Phys. Rev. Lett. 101, 226401 (2008).

[2] P. Piekarz, K. Parlinski, and A. M. Oleś, Phys. Rev. Lett. 97, 156402 (2006).

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