New discoveries in old magnetite

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Magnetite, first magnetic material discovered in Ancient Greece, is a ferrimagnetic spinel with anomalously high Curie temperature 850 K. Hence, it is viewed as an ideal candidate for room-temperature spintronic applications. It still attracts great attention due to puzzling properties of the Verwey transition that occurs at T = 124 K and is associated with a drop of electric conductivity [1] and a complex structural phase transition [2].

Our theoretical studies based on the LDA+U method demonstrated a strong interplay between the local electron correlations on Fe atoms and electron-phonon coupling, which plays a crucial role in the Verwey transition [3,4]. These results were confirmed by the inelastic x-ray scattering measurements at the ESRF in Grenoble that found anomalous, nonlinear broadening of low-energy phonons with decreasing temperature above the Verwey transition [5]. By a combination of these experimental results with ab initio calculations we revealed a strong anharmonicity induced by electron-phonon coupling. This anharmonic behavior is connected with the short-range fluctuations inherited from the long-range charge-orbital order observed below the Verwey transition [2].

Our recent diffuse scattering studies discovered very rich pattern in large areas of reciprocal space, which allows us to link the nature of short-range ordering with the long-range structure of the low-temperature phase [6]. It shows that whatever the electron localization pattern is, it partially survives up to room temperature as short-range correlations in the high-temperature cubic phase. Additionally, ab initio calculations reveal that characteristic features in the diffuse scattering pattern can be correlated with the Fermi surface topology.

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