Probing the lattice dynamics of nickel oxide across magnetic phase transition using X-ray absorption spectroscopy

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At room temperature, nickel oxide (NiO) is an antiferromagnetic Mott-Hubbard insulator, a compound that possesses a NaCl-type structure with slight rhombic distortion due to antiferromagnetic ordering [1], and an optical band gap of 3.7 eV [2]. Moreover, among all transition metal monoxides, NiO has the highest magnetic phase transition temperature, T_N = 525 K, from antiferromagnetic to paramagnetic states [3]. This implies that the material can ensure the magnetic stability of data carriers at temperatures significantly higher than room temperature. Additionally, NiO finds widespread applications in semiconductors, the electronics industry, rechargeable batteries, sensors and detectors, as well as in catalysis and pharmacy [4, 5].

In this study, we investigated the lattice dynamics of polycrystalline stoichiometric NiO across a wide temperature range, from 10 K to 900 K, both below and above the magnetic phase transition at T_N = 525 K. Additionally, we examined the lattice dynamics of polycrystalline non-stoichiometric NiO, where no phase transition is observed, and nanocrystalline NiO in the form of an aerogel. The temperature dependencies of the partial Ni-O and Ni-Ni radial distribution functions (RDFs) were obtained from the Ni K-edge extended X-ray absorption microstructure (EXAFS) spectra using the reverse Monte Carlo (RMC) method [6]. Furthermore, we determined the temperature dependencies of the mean-square relative displacement (MSRD) values for Ni-O and Ni-Ni atomic pairs by decomposing the respective RDFs into a set of Gaussian functions.

We found that the magnetic phase transition from the antiferromagnetic to paramagnetic phase in polycrystalline stoichiometric NiO is accompanied by a change in the rate of increase in MSRD as the temperature increases. However, such behaviour was not observed in the non-stoichiometric polycrystalline NiO sample.

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