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PRESSURE-INDUCED PHASE TRANSITIONS IN THE CoFe2O4 AND Zn0.34Fe2.53[]0.13O4 FERRITES

Bulk and nanostructured ferrites with a spinel-type crystal structure (AFe2O4) have been actively studied for many decades due to their attractiveness from both fundamental and practical points of view. Such compounds exhibit a wide range of physical phenomena: high electrical resistivity, low electrical losses, high chemical stability, magnetic phase transitions of various types, geometric frustration effects, and much more. This makes possible the wide technological application of ferrites as materials for transformers, solar cells, biomedicine, magnetic sensors, catalysts, drug delivery systems, electronic and magnetic components.

Depending on the chemical composition and size of nanoparticles, ferrites with a spinel structure have different distributions of cations in tetrahedral (A) and octahedral (B) oxygen coordination. In particular, the case can be realized when Fe3+ ions are in positions A, and there is also a mixture of Fe3+ and Fe2+ ions located in positions B. When doping with transition metals or alkali elements in positions A or B or creating vacancies in the cubic spinel structure, magnetic interactions between iron ions change. This leads to significant changes in the physical properties of these ferrites. It should be noted that changes in the physical properties of the material can be achieved by applying high pressure. Pressure causes a controlled adjustment of interatomic distances and bond angles, which leads to changes in the physical properties of ferrite oxides.

We have studied the crystal structure and vibrational spectra of bulk CoFe2O4 ferrite and Zn0.34Fe2.53 \boxtimes 0.13O4 cation-deficient nanostructured zinc ferrite (where \boxtimes denotes the cation vacancies) by means of the X-ray diffraction and Raman spectroscopy methods under high pressure.

The Zn0.34Fe2.53⊠0.13O4 compound has been studied in the pressure range of 0-34 GPa. At pressures above 18 GPa, a structural phase transition has been detected from the initial cubic phase with space group Fd3⁻m to the orthorhombic structure Bbmm. A feature of the phase transition in this compound is a wide range of phase coexistence pressures. Under pressure there is a gradual suppression of the initial cubic phase and an increase in the volume fraction of the orthorhombic phase. We have analyzed the dependences of unit cell parameters, bond lengths, and vibrational modes on the pressure. It has been revealed the influence of cation vacancies on the pressure dependences of the structural parameters of Zn0.34Fe2.53[]0.13O4 ferrite.

The CoFe2O4 compound has been studied in the pressure range from 0 to 35 GPa. We have found the structural phase transition from the initial cubic phase with space group Fd3⁻m to the orthorhombic structure Bbmm at the pressure of ~22 GPa. The two-phase state is observed in the pressure range from 22 GPa to 30 GPa. There is only the post-spinel phase in this compound above the 30 GPa, Near the phase transition, anomalies are observed in the dependence of vibrational modes on pressure. The lattice parameters, bond lengths, and bulk modulus have been determined for both the cubic and orthorhombic phases in this ferrite.

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Section

Energy and materials science (Section 2)

Primary author: RUTKAUSKAS, Anton (Frank Laboratory of Neutron Physics of Joint Institute for Nuclear Research)

Co-authors: Dr ZHALUDKEVICH, Alexander (Scientific-Practical Materials Research Centre of the National Academy of Sciences of Belarus); Dr KOZLENKO, Denis (Joint Institute for Nuclear Research); Mr LUKIN, Evgeniy (Joint Institute for Nuclear Research); Mrs LIS, Olga (Joint Institute for Nuclear Research); Dr KICHANOV, Sergey (Joint Institute for Nuclear Research)

Presenter: RUTKAUSKAS, Anton (Frank Laboratory of Neutron Physics of Joint Institute for Nuclear Research)

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