m36.p08

Sound wave velocities of Fe-Ni alloy at high pressure and temperature

Anastasia Kantor[a], Leonid Dubrovinsky[a], Innokenty Kantor[a], Alexander Kurnosov[a], Alexei Kuznetsov[a], Natalia Dubrovinskaia[b], Michael Krisch[c]

[a]*Bayerisches Geoinstitut, Universitaet Bayreuth, Germany.* [b]*Lehrstuhl fuer Kristallographie, Physikalisches Institut, Universitaet Bayreuth, Germany.* [c]*ESRF, Grenoble, France. E-mail: Anastasia.Kantor@uni-bayreuth.de*

Keywords: elastic properties, high-pressure, iron-nickel alloy

Knowledge of high-pressure and high-temperature elasticity of Fe-Ni alloy with low (5-25%) Ni content is crucial for geosciences since it is probably the major component of the core of the Earth, Mars, Mercury, Moon, satellites of Saturn and Jupiter. High-pressure and high-temperature (up to 41 GPa and 700 K) study of FeNi alloy with 22% of Ni was carried out by mean of inelastic X-ray scattering (IXS) from polycrystalline material. Two sets of experiments: at room temperature and at 700 (10) K have been performed. Before and after every measurement (taking about 10 hours) an *in-situ* 1-D monochromatic X-ray diffraction pattern was collected for volume determination exactly from the sample. X-ray diffraction study revealed stability of *fcc* over *hcp* phase in the whole studied *P,T* range. Isothermal equation of state was derived at room temperature and at 700 K. X-ray inelastic scattering measurements allow to calculate longitudinal acoustic wave velocity V_L, that gives, combined with measured equations of state, full isotropic elasticity of the material. We did not observe strong deviations from elastic properties of pure *hcp* iron. Recently reported for pure Fe high-temperature deviations from the Birth law [1] were not observed in FeNi alloy.

[1] Lin J.-F., Sturhahn W., Zhao J., Shen G, Mao H.K., Hemly R.J., *Science* 308, 1892-1894, 2005.

m36.p09

High-Pressure Structural, Electronic and Magnetic Transformations in Compound Iron Oxides

I.S. Lyubutin, A.G. Gavriliuk

Shubnikov Institute of Crystallography, Russian Academy of Sciences, 119333 Moscow, Russia. E-mail: lyubutin@ns.crys.ras.ru

Keywords: high pressure phase transformations, magnetic oxides, synchrotron radiation method

The high-pressure experiments in diamond anvil cells have been performed with several iron oxides having different crystal structures. The cubic yttrium iron garnet $Y_3Fe_5O_{12}$, the perovskite-like rare-earth orthoferrites $RFeO_3$ (R = Nd, Lu, Y) and multiferroic $BiFeO_3$ crystals, the hematite Fe_2O_3 with corundum structure, the rhombohedral iron borates $FeBO_3$ and trigonal rare-earth borate $GdFe_3(BO_3)_4$, were studied under high pressures up to 150 GPa. The single crystals enriched with Fe-57 isotopes have been prepared for nuclear resonance measurements. The Mössbauer transmission and Mössbauer synchrotron (NFS) spectroscopes, X-ray diffraction and the synchrotron high-resolution Kβ X-ray emission spectroscopy (XES), optical absorption spectroscopy, Raman scattering, electron microscopy, and electro-resistivity measurements have been applied. The sharp transformations in the crystal structures, in magnetic, electronic and spin states were discovered in several crystals at pressures of about 40-50 GPa. In $FeBO_3$, $RFeO_3$ and $BiFeO_3$, the X-ray spectra indicate the structural phase transition of the first-order type with a sharp drop of the unit cell volume. In $GdFe_3(BO_3)_4$, two crystal structure transitions at 26 and 43 GPa were observed. In the iron garnet $Y_3Fe_5O_{12}$, the transitions to an amorphous-like state was found at 49 GPa. In all investigated crystals the transitions from the magnetic to a nonmagnetic state were found in the critical region of pressures. The Mössbauer, optical and XES spectra indicate that the magnetic collapse is accompanied by transformations in electronic and spin structures of iron ions. This is explained by spin crossover in 3d electron system with the transition of Fe^{3+} ions from the high-spin (S = 5/2, $^6A_{1g}$) to the low-spin (S = 1/2, $^2T_{2g}$) state. The pressure dependences of the Neel temperature and the magnetic hyperfine field at iron nuclei H_{hf} were found and P(T magnetic phase diagrams were plotted for several crystals. It was established from the behavior of the optical absorption edge and from direct electro-resistivity measurements that in the $FeBO_3$, $RFeO_3$ and $GdFe_3(BO_3)_4$ crystals, the transition from the insulating to a semiconducting state takes place at the critical pressures. In $Y_3Fe_5O_{12}$ and $BiFeO_3$, the insulator-metal transitions were discovered. This is explained by the Mott-Hubbard type transitions with the extensive suppression of strong d-d electronic correlations. As to magnetic behavior, the low-spin state of Fe^{3+} in the high-pressure phase is not diamagnetic, and the low-temperatures synchrotron Mössbauer measurements of $FeBO_3$ indicate the magnetic correlations related to magnetic ordering of Fe^{3+} ions in the low-spin system. The magnetic ordering temperature of the low-spin Fe^{3+} ions was valuated, and P – T magnetic phase diagrams were plotted. The proposed theoretical consideration explains some details of the high-pressure magnetic properties. Several theoretical approaches for explanation of the observed transitions are discussed in connection with the breakdown of strong d-d electronic correlations. This work is supported by Russian Foundation for Basic Research grant N° 05-02-16142-a and by the Program of Russian Academy of Sciences ″Strongly correlated electronic systems″.