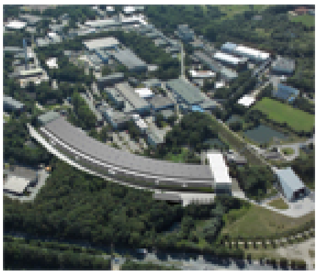

Contribution ID: **11**   Type: **not specified**

Structural, magnetic and electronic transitions in 3d-metal oxides under super high pressures

Tuesday 19 May 2009 11:15 (45 minutes)

Transition metal oxides constitute a very large class of materials of considerable importance for both fundamental science and practical applications. They include high temperature superconductors, manganites with colossal magneto-resistance, multiferroics, materials for spintronic and optoelectronic applications. Moreover, mixed iron oxides and perovskites are very important for geophysics. The properties and behavior of transition metal oxides are mainly governed by strong electron-electron correlations. In these systems many theories predict the pressure-induced insulator-metal phase transition which is accompanied by a collapse of the localized magnetic moment and a structural phase transition. However, until recently such scenario was not observed experimentally, since the expected values of necessary pressures exceed 2 Megabar.
We present the complex studies performed at super high pressures up to 200 GPa in diamond anvil cells using several experimental methods: Mössbauer transmission spectroscopy and Mössbauer synchrotron spectroscopy (Nuclear Resonance Forward Scattering –NFS), X-ray diffraction and synchrotron high resolution X-ray emission Fe-K⊠ spectroscopy (XES), optical absorption spectroscopy and direct measurements of electric resistance. The materials with different crystal structures, such as nickel monoxide NiO and magnesiowüstite (Mg,Fe)O), iron oxide Fe2O3, rare-earth orthoferrites RFeO3 (R = Nd, Lu, Y), yttrium iron garnet Y3Fe5O12, iron borates FeBO3 and GdFe3(BO3)4, multiferroic BiFeO3 and manganites LaMnO3 and MnFeO4 have been studied.
The transitions from the magnetic to a nonmagnetic state (magnetic collapse) was discovered in all crystals at pressures of about 40-55 GPa. The magnetic collapse is accompanied by a transformation of electronic and spin structures due to the spin crossover in 3d electron system at the transition of Fe3+ ions from the high-spin S = 5/2 (HS) to the low-spin S = 1/2 (LS) state. At the same pressures, the structural phase transitions with a sharp drop of the unit cell volume were found in several crystals. We have established that the metallization process is very complicated. In the pressure region of the HS-LS spin crossover, many crystals are transformed from the dielectric to a semiconducting state. The direct insulator-metal transition (IMT) was found in Y3Fe5O12 and BiFeO3 crystals. These effects are explained by the Mott-Hubbard type transitions with the extensive suppression of strong d-d electronic correlations.
A new mechanism of the insulator-metal transition in Mott-Hubbard insulators was found. This new mechanism can be initiated by high pressure and it is driven by the spin-crossover of d5 ions from HS to LS state. The spin-crossover suppresses the Coulomb correlation energy Ueff down to the value enabling the insulator-metal transition according to the Mott mechanism Ueff/W ≈ 1 (W is the half bandwidth). Such type of Mott metallization was observed experimentally in multiferroic BiFeO3. We call the new IMT mechanism as the "Hubbard energy control" mechanism, to distinguish from the well known "bandwidth control"and "band-filling"mechanisms of the IMT.
Supports by RFBR (Grants № 08-02-00897a and № 07-02-00490-a) and by the RAS Program "Strongly correlated electronic systems"are acknowledged.

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Session Classification: Dynamic Single Crystal Diffraction at simultaneous high-pressure and -temperatures