

s5.m16.o4 **Crystallographic Transitions Related to Magnetic and Electronic Phenomena Under High Pressure in Iron Oxides and Compounds.** G. Kh. Rozenberg^a, M. P. Pasternak^a, L. S. Dubrovinsky^b ^a*School of Physics and Astronomy, Tel-Aviv University, Ramat-Aviv, 6997, Tel Aviv, Israel,* ^b*Bayerisches Geoinstitut, University Bayreuth, D-95440 Bayreuth, Germany. E-mail: emtsm@post.tau.ac.il*

Keywords: High Pressure; Crystallographic Transition; Magnetic/Electronic Transitions

The main objective of this paper is the study of structural aspects of strongly correlated systems in conjunctions with magnetic/electronic properties in a regime of matter under very high density. Synchrotron X-ray diffraction (XRD) measurements were carried out to 130 GPa to probe structural features specifically related to pressure-induced (PI) magnetic/electronic transitions in selected transition metal (TM) compounds, emphasizing those with geophysical interest. The types of electronic transitions discussed are the *Mott transition* (MT), and *high-spin* (HS) to *low-spin* (LS) crossover. In these cases the electronic transition may induce or be a consequence of structural alterations. For instance a first-order PI spin-crossover will be accompanied by an abrupt reduction of the TM ionic-radius, hence by a discontinuous volume decrease. On the other hand a “sluggish” or second-order spin-crossover may result in non-linear crystal elastic constants which will affect the *equation of state*. In case of a MT, a fundamental electronic process in which a strongly correlated magnetic-insulating system becomes non-magnetic and metallic, one expects major modifications of the lattice parameters or even structural symmetry changes.

As example-cases we present results in Fe₂O₃, Fe₃O₄, FeI₂, FeCr₂S₄, and the RFeO₃ orthoferrites (R=rare earth).

These studies allowed us to:

- Establish typical structural features specific to *Mott-Hubbard* or *Charge-Transfer* electronic transitions.
- Obtain information about the PI structural changes due to the degradation of the magnetic state caused by the HS-LS transition.
- Elucidate the impact of these phenomena on particular crystallographic phase transitions, contribution of inelasticity to the equation of state of the new HP-phases, and on the classification of the phase transition orders (1st or 2nd order).

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s5.m16.o5 **High-pressure Behavior of Pyroxenes.** Tiziana Boffa Ballaran^a, ^a*Bayerisches Geoinstitut Bayreuth, Germany. E-mail: tiziana.boffa-ballaran@uni-bayreuth.de*

Keywords: Pyroxene; High-Pressure Single-Crystal X-Ray Diffraction; Phase Transitions

Pyroxenes (general formula M₂M₁T₂O₆) comprise approximately 25% of the Earth's volume to a depth of about 400 km. They have been the subject of many studies not only because of their abundance but also because of the variety of polymorphs and complicate phase transitions as a function of temperature, pressure and composition. The general topological features of pyroxenes can be described by the stacking sequences of octahedral (M1) and tetrahedral (T) layers, with M2 atoms lying between the bases of opposite tetrahedra and having different coordination depending on temperature, pressure and chemistry. Among the pyroxenes, the (Mg,Fe)SiO₃ join is of particular interest due to the importance of Mg and Fe substitution which is a common feature of all minerals of the Earth's mantle. Under compression the low-clino *P2₁/c* polymorphs of enstatite (MgSiO₃) and ferrosilite (FeSiO₃) undergo transitions to phases having *C2/c* symmetry [1-3]. Substitution of other elements at both M sites of the clinopyroxene structure affects substantially the transition with possible consequences for upper-mantle discontinuity structures. One of the most important cation substitutions is that of Ca since it occurs in most mantle clinopyroxenes. Knowledge about its influence on the high-pressure *P2₁/c* to *C2/c* phase transformation of clinopyroxenes is necessary in order to better constrain the thermodynamic properties of natural pyroxenes. The presence of Ca into the (Mg,Fe)SiO₃ structure causes a decrease of both the transition pressure and the hysteresis associated with the phase transition. The major structural changes associated with the transition are relative to the kinking of the tetrahedral chains and to the bond distribution involving the M2 atoms.

- [1] Angel, R. J., Chopelas, A. & Ross, N. L. (1992). *Nature* **358**, 322-324.
- [2] Hugh-Jones, D. A., Woodland, A. B. & Angel, R. J. (1994). *Am. Min.* **79**, 1032-1041.
- [3] Ross, N. L. & Reynard, B. (1999). *Eur. J. Min.* **11**, 585-589.