ESRF	**Experiment title:** HIGH PRESSURE CRYSTALLOGRAPHIC CONSEQUENCES OF ELECTRONIC AND MAGNETIC TRANSITIONS IN MOTT INSULATORS.	**Experiment number**: HS1906
Beamline: ID09A	**Date of experiment**: from: 11.12.02 to: 15.12.02	**Date of report**: 18.02.04
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Report:

Y. Amiel, G. Kh. Rozenberg, M. P. Pasternak, N. Nissim, A. Sani, ***Pressure-Induced Electronic and Structural Transformations in $FeCr_2S_4$,*** **submitted to Phys. Rev. B**

ABSTRACT

Electronic and structural properties of the ferrimagnetic semiconductor $FeCr_2S_4$ were determined by combining the methods of electrical resistance, R(P,T), ^{57}Fe Mössbauer spectroscopy, and synchrotron x-ray diffraction, to 20 GPa using diamond anvil cells. It was found that a local maximum on R(T) curve, corresponding to the CMR effect, substantially diminishes and broadens with pressure increase shifting to higher temperatures and finally disappears at ~7 GPa. Suppressing of the CMR effect corroborates with a trend toward gap closure resulting in a breakdown of the electronic *d-d* correlation, leading to a *Mott* transition, e.g., to a metallic and a non-magnetic Fe^{2+} electronic state. The Mott transition is

accompanied by an appreciable volume decrease of ~5% and gives rise to a sluggish first-order phase transition from spinel to Cr_3S_4-like structure accompanied by an additional ~13% volume collapse. The structural transition is completed at ~ 15 GPa. The relations between the structural and the electronic transitions are discussed.

G. Kh. Rozenberg, M. P. Pasternak, W. M. Xu, L. S. Dubrovinsky and S. Carlson,
High-Pressure Structural Phase Transition with no Symmetry Change Induced by High – Low Spin Crossover in $RFeO_3$ Perovskites, **will be submitted to Phys. Rev. Lett.**

ABSTRACT

High pressure synchrotron x-ray diffraction studies to 120 GPa and Raman studies up to 60 GPa were carried out in the antiferromagnetic RFeO$_3$ perovskites with representative rare-earth cations R starting with the *larger* Pr^{3+}, *intermediate* Eu^{3+} to the *smallest* Lu^{3+}. The XRD and Raman spectroscopy data have been analyzed taking in account the recent results of ^{57}Fe Mössbauer spectroscopy. It was found that all RFeO$_3$ undergo almost reversible first-order isostructural phase transition around 50 GPa accompanied by a significant and abrupt volume shrinkage (4-6.4%). For the larger and intermediate R the volume collapse concurs with a substantial reduction of the distortion of the orthorhombic unit cell while for the smaller Lu a "pure" isostructural transition is observed. It was concluded that all these transitions are driven by the high-to low spin transition (HS-LS) in Fe^{3+} namely, $S=5/2$, $^6A_{1g}$ → $S=1/2$, $^2T_{2g}$ and represents a new kind of pressure-induced **isostructural** transitions driven solely by spin state changes. The sluggish second-order HS-LS transition accompanying the first order isostructural phase transition in $PrFeO_3$ is reflected in its EOS due non-linear elastic constants.