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Pressure Induced Structural Changes in Nano-sized Materials Studied with On-Line Brillouin Spectroscopy and XRD. V.B. Prakapenka[a], I. Kantor[a], A. Kantor[b], S. Sinogeikin[c], M.L. Rivers[a], S.R. Sutton[a]. [a]*CARS, University of Chicago, USA.* [b]*Bayerisches Geoinstitut, Germany.* [c]*HP-CAT, Carnegie Institution of Washington, USA.*
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The combination of Brillouin spectroscopy (BS) with x-ray diffraction (XRD) was shown to be very effective in the high pressure studies of single crystals in the diamond anvil cell [1]. However, in a number of cases, high pressure induced, single crystal re-crystallization due to phase transition and stress significantly limited the high pressure-temperature range suitable for reliable BS and XRD measurements. In this work, we present a new approach in high pressure research employing the combination of BS with synchrotron XRD for characterization of nano-sized materials that could be readily synthesized in-situ at high pressure [2]. The main reasons for using nano-structural materials are to (1) reduce the anisotropy of samples probed with BS/XRD and (2) avoid significant effects on the Brillouin spectra due to the high sensitivity of acoustic velocities to crystallographic direction. The ability to perform simultaneous measurements of velocities and bulk modulus Ks (by BS), and the volume/density (by XRD) independent of any pressure standard in the same pressure-temperature environment provides essential information to resolve discrepancies between experimental data and theoretical calculations. The advantages and excellent performance of this technique will be illustrated by the characterization of elastic and structural properties of nano-sized ZnO at the pressure induced phase transition from hexagonal (wurtzite, B4) to cubic (rock salt, B1) phase.

[1] Sinogeikin S., Bas J., Prakapenka V.B. et al, *Rev. Sci. Instrum*, **2006**, 77, 103905. [2] Prakapenka V.B., Shen G.Y., Rivers M.L. et al, *J. Syn. Rad.*, **2005**, 12, 560.

Keywords: nano-crystallography; brillouin spectroscopy; high pressure

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High-Pressure Studies of Transition Metal Compounds Located Near the Insulator-Metal Borderline. Karl Syassen. *Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany.*
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Experimental high pressure studies of crystalline phases take advantage of numerous recent developments in diamond-anvil-cell techniques. Major advances have occurred in microscopic analytical methods that utilize synchrotron x-ray radiation (diffraction and inelastic scattering), optical spectroscopies, and synchrotron infrared spectroscopy. Concerning correlated electron systems, the subjects of interest range from pressure-induced structural changes to illuminating the interplay between more subtle changes in atomic arrangements, electron delocalization, magnetism, and superconductivity. Some recent results will be highlighted in this presentation. The main focus will be on structural and electronic properties of perovskite-related transition metal oxides located near the insulator-metal borderline, specifically titanates and vanadates. New findings for cuprate superconductors and Fe-based pnictides will be addressed briefly.

Work performed in collaboration with X. Wang, I. Loa, S. Karmakar, I. Efthimiopoulos (MPI/FKF Stuttgart), M. Hanfland, M. Merlini (ESRF Grenoble), and Y.-L. Mathis (ANKA Karlsruhe).

Keywords: transition metal oxides; high-pressure; X-ray diffraction

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Pressure-Induced Crystallographic Transitions Related to Electronic/Magnetic Phenomena in Iron(II,III) Compounds*. Gregory Kh. Rozenberg[a], Moshe P. Pasternak[a], Weiming M. Xu[a], Alexander Kurnosov[b], Leonid S. Dubrovinsky[b], Sakura Pascarelli[c], Manuel Munoz[c], Marco Vaccari[c], Michael Hanfland[c]. [a]*School of Physics and Astronomy, Tel-Aviv University, Ramat-Aviv, 6997, Tel Aviv, Israel.* [b]*Bayerisches Geoinstitut, University Bayreuth, D-95440 Bayreuth, Germany.* [c]*European Synchrotron Radiation Facility, BP 220, 38043 Grenoble Cedex, France.*
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The main issue of this paper is structural aspects of electronic/magnetic transitions in iron (II, III) compounds in a regime of very high static density. The experimental tools used were (a) synchrotron X-ray diffraction (XRD) as a structural probe (b) Mössbauer spectroscopy with its hyperfine interactions as magnetic probes, (c) electrical resistivity as a tool to identify gapped or gapless states, and (d) *K*-edge X-ray absorption spectroscopy as an atomic-scale structural and valence state probe. We concentrated on the following phenomena and corresponding structural transformations:
(i) PI metal–metal *intervalence charge transfer* in the layered antiferromagnetic $Cu^{+1}Fe^{3+}O_2$ delafossite as a result of the increase in overlap of atomic orbitals. This process results in part of the Fe^{3+} converting into Fe^{2+} concurrent with $Cu^{1+} \rightarrow Cu^{2+}$ partial transition with the creation of the new Cu^{2+} - Fe^{2+} magnetic sublattice. XRD studies have shown a sequence of *R-3m* → *C2/c* → *P-3m* structural phase transitions at the 18 – 30 GPa range leading to the breakage of the dumb-bell like O-Cu-O bonds and formation of a CuO_4 tetrahedral. This results in the stabilization of the antiferromagnetic order and further culminates into the discussed valence transformation. The transitions are completely reversible in pressure and with no noticeable hysteresis. This pressure-induced sequence of structural phase transitions, the first triggered by the structure instability of *R-3m* beyond 18 GPa and the second by the electronic overlap of the Cu and Fe *d*-bands adds