s6.m1.o1 **Recent developments in the realization of a practical pressure scale for extreme conditions.**
W.B. Holzapfel, *FB Physik, University of Paderborn, 33095 Paderborn, Germany*
Keywords: extreme conditions.

Theoretical constraints on the analytic forms for the representation of equations of state for "regular" solids together with new critical inspections of available shock wave data, new constraints on the Grüneisen parameters, and the use of accurate ultrasonic data for the bulk moduli result in the realization of a practical pressure scale, which uses equations of state of some calibrants like Cu, Ag, and Au, and allows for realistic estimates of the uncertainties related to this pressure scale even under extreme conditions and not only at ambient temperature but also in wide ranges of temperature from OK up to the relevant melting curve. These new data will be compared with previous pressure scales based on the same calibrants.

s6.m1.o2 **Advances in high-pressure experiments combining XAS, temperature scans, and ESXD.**
A. Filipponi[1], J. P. Itiè[2], A. Di Cicco[3], [1]*INFM and Dip. Di Fisica, Università L' Aquila, Italy,* [2]*LPMC, Univ. Paris 6, 2 place Jussieu, Paris, France,* [3]*INFM and Dip. di Matematica e Fisica, Universitá di Camerino, Camerino (MC), Italy*
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The availability of high-brilliance tunable hard x-ray beams at the European Synchrotron Radiation Facility, or other third generation synchrotron radiation sources, has opened new opportunities for x-ray absorption spectroscopy (XAS) investigation in the high-pressure field. At the ESRF-BM29 XAS beamline we have developed[1] and recently exploited novel experimental techniques suitable for high-pressure high-temperature studies using the Paris-Edinburgh press or other high-temperature devices. This experimental station combines XAS with x-ray absorption temperature scans, and energy scanning x-ray diffraction (ESXD). Temperature scans are performed by ramping the heating power of the sample oven at the desired speed. From the observation of the changes in the x-ray absorption coefficient at constant energy (chosen at significant points, to enhance structural or electronic sensitivity) it is possible to reveal the occurrence of phase transitions (solid-solid, melting ...) and to access important physical properties such has the nucleation rate of the stable crystalline structures in an undercooled liquid or the liquidus curve in eutectic binary phase diagrams. X-ray diffraction, which is essential for pressure calibration and sample diagnostic, is detected using a fixed angle high-resolution collimator. With this detection method it is possible to reach a sensitivity of 10^{-4} in lattice spacing determinations. The q-scan is performed through a monochromator energy scan[1].

With such a unique setup, which combines experimental techniques sensitive short and long-range structural properties, it is possible to study condensed matter in the liquid and solid phases in a wide pressure and temperature range (P=0.2-10 GPa and T=300-1500 K). Recent applications to pure Ge and Ag:Ge alloys will be presented.

[1] A. Filipponi, M. Borowski, D. T. Bowron, S. Ansell, S. De Panfilis, A. Di Cicco, and J.-P. Itiè, Rev. Sci. Instr. (to be published, 2000).

s6.m1.o3 **Structural transitions related to magnetic phenomena under high pressure.** G.Kh. Rozenberg, M.P. Pasternak, *School of Physics and Astronomy, Tel Aviv University, Ramat Aviv, 69978 Tel Aviv, Israel*.
Keywords: extreme conditions.

In recent years *3d* transition metal (TM) compounds (*Mott Insulators*) have been the focus of intensive basic research in materials science. Notable cases are studies of high-T_C superconductivity in doped rare-earth copper-oxides and of unusual magneto-resistance effects in doped manganese TM-oxides. A remarkable experimental observation pertinent to the nature of those strongly correlated systems has been the unambiguous discovery of the elusive Mott transition induced by pressure[1]. The Mott transition comprises an insulator-metal (IM) transition concurrent with the collapse of TM ion magnetic moments. It can be accompanied by a slight volume reduction due to electron delocalization.

Another important mechanism related to magnetism at high-pressure is the degradation and even complete collapse of the magnetic state due to *spin-crossover*: a high-spin (HS) to low-spin (LS) transition, a result of Hund's rule breakdown at very high density[2]. Such a transition will be accompanied by a significant reduction of the TM ionic radii therefore volume decrease or even structural changes.

In the above-mentioned cases the electronic transition prompts structural alterations, but *visa versa*, it is also possible that a structural phase transition will induce a *Mott* or HS-LS transition.

In this paper we discuss both type of pressure-induced transformations: *i*) structural changes resulting from magnetic/electronic phase transitions, and *ii*) magnetic/electronic changes resulting from crystallographic phase transitions. Using diamond anvil cells the following experimental tools are used: (a) **Synchrotron X-ray diffraction** for probing crystallographic phase transitions and detailed structural changes at the vicinity of the *Mott* and or HS-LS transitions, (b) **Mössbauer spectroscopy** as atomic-scale structural and magnetic probe, and (c) **electrical resistivity** as a tool to identify gapped or gapless states and features of the IM transition. As examples cases we present recent and previous results in Fe_2O_3, FeI_2, $FeCl_2$, and the $R$$FeO_3$ orthoferrites.

[1] Pasternak M. P., Taylor R. D., Chen A., Meade C., Falicov L. M., Giesekus A., Jeanloz R., and Yu P. Y. « Pressure-induced metallization and the collapse of the magnetic state in the antiferromagnetic insulator NiI2. », Phys. Rev. Lett., (1990), **65**: 790-793
[2] Pasternak M.P., Taylor R.D., Jeanloz R., Li X., Nguyen J.H., McCammon C.A., «High pressure collapse of magnetism in $Fe_{0.94}O$: Mössbauer spectroscopy beyond 100 GPa.», Phys. Rev. Lett., (1997), **79**: 5046-5049.

s6.m1.o4 **Low temperature structural studies of molecular crystals under pressure. X-ray diffraction equipment for (P+T) phase diagram investigations**. Y. Barrans, J. Gaultier, D. Le Pevelen, P. Guionneau, D. Chasseau, *Institut de Chimie de la Matière Condensée de Bordeaux, CNRS UPR 9048, 87 Av. Dr A. Schweitzer, 33608 Pessac Cedex, France.*
Keywords: extreme conditions.

The coupling of our high pressure and our low temperature techniques has been performed and tested on organic conductors: we can now reach any point of the phase diagram. We use a classical monochromatized X-ray source (CuKα for films, MoKα for intensity collection), a diamond anvil cell (pressure) fixed on a vertical closed cycle He cryostat (low temperature) and isolated with a pair of containers. The X-ray beams cross essentially Be walls in a 35° half aperture cone. A radial collimator suppresses nearly all the scattering from the containers on the patterns, and a careful screening of the background and peaks is performed for the collected intensities. Using normal beam geometry the Gaultier vertical Weissenberg camera gives informations on the reciprocal space and the Gaultier Huber three circle diffractometer allows full data collection. The possibilities of both systems will be illustrated through examples of investigations down to 7 K and up to 14 kbar.

Notes

s6.m1.o5 Structure of Liquids at High Pressure Probed by X-ray Diffraction. M. Mezouar, S. Bauchau, G. Blattman, *ESRF, B.P. 220, 38000 Grenoble*
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The determination by *X*-ray diffraction of the evolution at high pressure and high temperature of inter-atomic distances, and number of first neighbors of disordered systems (liquids, amorphous materials), is of great importance in various domains such as material science or geophysics. In particular, it has been recently shown that liquids exhibit under high pressure a much more complex behavior than previously expected. For instance, a first order phase transition (sharp transition with large volume change) that are usually only observed in the solid state has been clearly evidenced in liquid phosphorus. More generally, it is remarkable that the structural relations between polymorphs in the solid and in the liquid state is poorly understood. This lake of information on the structure of liquid at high pressure is mostly due to experimental difficulties : i.e. low and diffuse signal, high background, high chemical reactivity of liquid phases at high temperature. In order to overcome this difficulties a Soller slit system has been developed at beamline ID30, ESRF. Preliminary results on liquid tin obtained with this new device interfaced to the Paris-Edinburgh large volume press and a fast detector based on image-plates will be presented.