Experimental Research Related to HPCAT – APS

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During the year 2003 we have made 5 trips to HPCAT to perform experiments on 16ID-B. The first trip was in collaboration with Malcolm Nicol from UNLV. The following trips were made through CDAC.

The focus of these experiments has been two-fold. First, we have been studying a radial diffraction technique that allows us to examine the effects of deviatoric stress due to non-hydrostatic conditions. Radial diffraction, along with a properly designed diamond anvil cell (DAC), provides access to all stress angles, ψ. ψ is the angle between the reciprocal lattice vector of a d(hkl) plane and the compression axis. Fortunately, the stress-strain conditions within the sample environment of a DAC have been well-defined by A. K. Singh et al [1]. By combining the existing theoretical work and the experimental results from HPCAT there is a wealth of information that can be attained. The elastic constants, which are currently unknown at pressure, for various materials can be calculated. However, the governing equations are complicated so there is a practical limit to the structures one can derive the elastic constants for. Another parameter that can be determined is the hydrostatic $d_p(hkl)$. The equation related to this from Singh's work is

$$d_m(hkl) = d_p(hkl)[1 + (1- 3\cos^2 \psi)Q(hkl)].$$

$d_m(hkl)$ and $Q(hkl)$ are the measured d-spacing and a complicated function that depends on the properties of a particular material. By choosing the angle $\psi \approx 54.7$ degrees (the magic angle) the previous equation reduces to

$$d_m(hkl) = d_p(hkl).$$

The effects of the deviatoric stresses at this angle have been removed from the measured d-spacing thus providing a hydrostatic result. This leads to more accurate equation of state parameters, as well as, eliminating some of the controversy between various static experiments and dynamic experiments. We are still in the process of analyzing the data, however we have thus far seen errors in pressure and volume on the order of a few percent in high symmetry structures. The low symmetry structures possess errors on at least the same order, if not greater. The issue of deviatoric stress is more of a concern for the low symmetry structures because a small deviation in the $d_m(hkl)$ can lead to a different structure determination [2].

The second focus of our experiment has been to study lanthanides such as cerium in order to better understand f-electron behavior. There are many outstanding debates in cerium literature that make it a prime candidate to test magic angle x-ray diffraction, plus it contains large volume collapses and an iso-structural phase transition.

This research is leading us to a greater understanding of high pressure-temperature conditions by providing more information than can be attained by standard x-ray diffraction geometries and by providing more accurate EOS data.

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References:

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[2] G. N. Chesnut, B. D. Streetman, D. Schiferl, W. W. Anderson, M. Nicol and Y. Meng, to be published in Conference proceedings of the APS Topical Group on Shock Compression of Condensed Matter, July, 2003; Portland, OR