MS18.06.05 INTENSITY ANALYSIS FOR HIGH PRESSURE POWDER DIFFRACTION USING DIAMOND ANVIL CELLS. H. Fujihisa, K. Aoki, H. Yamawaki, and M. Sakashita, National Institute of Materials and Chemical Research, 1-1 Higashi, Tsukuba, Ibaraki 305, Japan

An angle dispersive powder x-ray diffraction experiment with an image plate (IP) and a diamond anvil cell has greatly improved data quality1, which allows us to get an accurate structure including atomic parameters under pressure. The use of the synchrotron beam is recommended to get high angular resolution and sufficient intensity in powder patterns. The IP makes it possible to remove geometrical error easily on computer and to generate a 2theta versus intensity pattern.

Then we can determine atomic parameters by the Rietveld or the least-square methods. A powder pattern of which structure is fully known also gives electron density distribution map. The limiting number of the observed peaks causes termination errors in both maps of the traditional Fourier synthesis and the previous maximum entropy method (MEM)2. To overcome this problem, we have developed a new MEM for high pressure experiments3 which can reduce the termination errors by the same theory as the difference synthesis.

References
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MS18.06.06 X-RAY DIFFRACTION OF LIQUIDS AND GLASSES AT HIGH PRESSURE. Willem L. Vos[1] and Marco J. P. Brugmans[2]. [1]van der Waals-Zeeman Instituut, Universiteit van Amsterdam, 1018 XE Amsterdam, The Netherlands; [2]FOM Instituut voor Atoom- en Molecuulfysica, 1098 SJ Amsterdam, The Netherlands

In contrast to crystals, the usual subject study of crystallography, the constituent atoms of liquids and glasses have random spatial positions. Nevertheless, there is still some degree of (local) order that can be described with statistical distribution functions, e.g. the radial distribution function g(r). This function is proportional to the probability of finding an atom at a distance r from a central atom. The Fourier transform of this function is the structure factor S(Q), that can experimentally be measured.

Structural studies of liquids and glasses at high pressure are very scarce, which is probably due to the experimental difficulties: the scattered signal from amorphous samples is much broader than crystalline diffraction peaks. Thus, the signal is weak and hard to distinguish from the background caused by the relatively large cell windows.

The use of high-brightnes synchrotron x-ray radiation is an obvious choice, because samples in high pressure environments are usually very small, and we are interested in systems consisting of light elements. In this talk, we will discuss several sources of systematic errors. The main experimental situation aimed at is monochromatic scattering in combination with image plates (Daresbury SRS 9.1). Comparisons will be made to position sensitive detectors and to polychromatic scattering detected with solid state detectors. Illustrations will be provided from our recent work on liquid and glassy methanol [1].

[1] M.J.P. Brugmans and W.L. Vos, J. Chem. Phys. 103, 2661 (1995), and to be published.

MS18.06.07 THE HIGH PRESSURE MENU. John B. Parise, Earth & Space Sciences, State University of New York, Stony Brook, NY 11794-2100

Technical Developments, in cell design, in brighter national and laboratory-based facilities, along with the availability of these to a broader range of researchers, bodes well for the continued vitality of high pressure science and its visibility.

This presentation will concentrate on the developments, new directions and research opportunities presented at the meeting. These remarks will emphasize the strengths and limitations of the current generation of hardware, software and methodologies.

PS18.06.08 TWO-DIMENSIONAL DIFFRACTION DATA COLLECTION WITH A LARGE-VOLUME PRESS AT THE NSLS. Jiuhua Chen, Rui Li, John B. Parise and Donald J. Weidner, Center for High Pressure Research (CHiPR) and Department of Earth and Space Sciences, State University of New York at Stony Brook, Stony Brook, NY 11794-2100

In situ structure determination and refinement is a growing trend in the highpressure diffraction community. To obtain this crystallographic information, accurate diffraction-intensity data combining with existing d- space data is indispensable. Combination of a two-dimensional detector, an imaging plate, with a DAC has shown a great potential in collecting the accurate intensity data.

To take the advantages of a large-volume press, a quasi-hydrostatic pressure environment, large amount of diffracting sample, easy heating, and low temperature gradients, the imaging plate was applied to the DIA-type apparatus SAM85 at the X17B beamline of NSLS at Brookhaven National Laboratory. A high-pressure cell assembly with a disk-type heater was designed to minimize the number of materials in the x-ray path, and a subtraction technique was applied to eliminate the extrinsic peaks and background from the diffraction pattern. Typical exposure time is 5 min. Powder diffraction experiments were carried out on Ni-Mg olivine and $NiAl_2O_4$ spinel samples aiming to obtain the site-occupation information in these crystals. Structure refinements based on these observed data showed a obvious favor ordering of the cation distribution in these systems at high pressure. A kinetic phenominon of cation redistribution was observed in solid solution system of Ni-Mg olivine at 800 C and 4 GPa in 70 min.