An angle dispersive powder x-ray diffraction experiment with an image plate (IP) and a diamond anvil cell has greatly improved data quality, 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 limited number of the observed peaks causes termination errors in both maps of the traditional Fourier synthesis and the previous maximum entropy method (MEM). To overcome this problem, we have developed a new MEM for high pressure experiments which can reduce the termination errors by the same theory as the difference synthesis.

References

MS18.06.06 X-RAY DIFFRACTION OF LIQUIDS AND GLASSES AT HIGH PRESSURE, Willem L. Vos and Marco J. P. Brugmans², Ivan der Waals-Zeeman Institut, Universiteit van Amsterdam, 1018 XE Amsterdam, The Netherlands; ²FOM Instituut voor Atom- en Molecuulphysica, 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-brightness 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].

References