

energy x-ray diffraction and diamond anvil cell techniques were used to study the structural evolution of powder and amorphous materials under pressure, as well as the time dependence of the crystallization procedure. These will provide new insight on the nature of phase transition, provide new invitation for the electronic theoretical studies for the phase stability, and improve our understanding of the kinetic process of the common pressure induced crystallization.

Keywords: high pressure, phase transition, high energy XRD

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#### Pressure-induced change of the chemical short-range order in liquid compounds

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To reveal the effect of chemical bonding character on the pressure-induced structural changes, we have investigated the structures of various tetrahedrally bonded materials, such as liquid group 14 elements, III-V, II-VI and I-VII compounds, under high pressure. The results have shown that these liquids show various high-pressure behaviors (local structures and the sharpness of structural changes), depending on the covalent/ionic character [1]. However, these results are based on the average structure, which does not differentiate the chemical component around each atom. To observe partial structures is inevitable to understand the nature of the various structural changes in liquid compounds. For this purpose, we have developed the method to determine the partial structure in liquid compounds at high pressures using an anomalous x-ray scattering method (AXS) and applied it to liquid AgI. The experiment was performed at a JAEA undulator beamline BL22XU in SPring-8. The high pressure and high temperature condition was generated with a multi-anvil high-pressure apparatus, SMAP180. The data was collected by an angular dispersive x-ray diffraction method using a solid state detector. The incident x-ray energy was tuned into the energies below 300 and 20 eV from the absorption edge of two constituents. The obtained partial structural functions are in good agreement with the results of ab-initio MD calculation [2], which supports the validity of the AXS method to investigate the chemical short-range order in the liquid compounds. [1] T. Hattori et al., PRB 68, 224106 (2003), T. Hattori et al., PRB 72, 064205 (2005), T. Hattori et al., PRB 73, 054203 (2006), T. Narushima et. al., PRB 76, 104204 (2007), T. Hattori et. al., PRB 76, 144206 (2007), [2] F. Shimojo, (private comm.)

Keywords: high pressure, liquid, anomalous x-ray scattering

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#### A method for analysis of energy-dispersive X-ray diffraction from disordered systems under pressure

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Energy-dispersive x-ray diffraction method is commonly used for x-ray diffraction measurements using a cubic-type multi-anvil-press

because good background elimination and short data acquisition time can be achieved simultaneously. However, diffraction intensity is affected by several energy-dependent factors, such as intensity spectrum of a synchrotron radiation source, sensitivity spectrum of a detector, absorption spectra of the sample and those of the surrounding materials. Because it is difficult to estimate these factors separately, Tsuji et al., proposed a new empirical method for determination of structure factor of liquids and glasses [1]. Furthermore, Funakoshi et al., developed a Monte Carlo simulation code to carry out the procedure [2]. But these analyses sometimes give unreasonable results. We improved the method by implementing a common normalization method in a new code. The obtained structure factors of silica glass and liquid water at ambient conditions agree well with those reported previously.

[1]K. Tsuji, et al., Rev. Sci. Instrum. 60 (1989) 2425.

[2]K. Funakoshi, Ph.D thesis, (1997, Tokyo Institute of Technology).

Keywords: liquid-state diffraction, high-pressure structure determination, energy-dispersive X-ray diffraction

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#### Pressure- and temperature-induced structural phase transition mechanisms of nitrogen

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A theoretical description is proposed for the pressure and temperature induced structural transitions of nitrogen. Three regions of the phase diagram are distinguished corresponding to different types of transition mechanisms and parent structures. Combined ordering and displacive reconstructive transitions are found in the lowest pressure region, from the parent disordered  $\beta$  structure to the ordered  $\alpha$  and  $\gamma$  structures. In a second region, which extends from about 2 to 140 GPa at room temperature, group-subgroup related structures occur, which realize ferroelastic or ferroelectric distortions of the parent  $\delta$  structure. Space-group symmetries, consistent with the assumed structural mechanisms, are proposed for the  $\delta_{loc}$ ,  $\zeta$ ,  $\kappa$ ,  $\iota$  and  $\theta$  molecular phases. Above 140 GPa, in the molecular dissociation region, the local structure of the  $\eta$  phase is assumed to realize a link between the molecular  $\zeta$  and  $\kappa$  phases and the high-temperature cg-N phase.

Keywords: nitrogen, phase transitions in solids, Landau theory

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#### Thermodynamic exploration of conformational space of 1,2-ethylene glycol

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Ethylene glycol (1,2-Ethanediol, EG) is wide by applied mainly as an anti-freezing additive, but also as a substrate and solvate in many industrial. Owing to the vicinal location of two hydroxyl groups (-OH) in this very simple molecule, EG serves as a model