The Structural Change near the Semiconductor-Metal Transition in Arsenic Chalcogenides

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Recent our EXAFS measurements [1-2] for liquid chalcogeneides such as As_xTe_{1-x} and As_xSe_{1-x} reveal that the threefold coordinated As sites rapidly decreases with increasing temperature, which suggests that the network structure formed by threefold As and twofold chalcogens transforms into the chain structure at high temperature. This structural transformation is accompanied by the transition from semiconducting to metallic state.

The main object of our project is to investigate the modification of the atomic arrangements in liquid chalcogenides near the transition from the microscopic point of view by utilizing the strong X-ray source in SPring-8. This may give helpful understanding on the strong correlation in liquid chalcogenides between the electronic states and atomic arrangements.

In order to extract the accurate structure factor from the observed scattering intensity, careful corrections have to be thought for each experiment. The important corrections for processing the data are as follows:

(1) Correction for the intensity of the backgrounds due to the sample and its container.
(2) Correction for temperature and angular variations of the inelastic and incoherent Compton scattering.
(3) Correction for the polarization of X-ray.
(4) Escape correction for the Ge detector.
(5) Determination of the density for irradiated sample part.

At first, we have started to measure the scattering intensity at different scattering angles and energies (1) for quartz glass and crystalline sapphire sheets both of which may be most suitable materials as liquid container at high temperature and pressure, and (2) for amorphous As_2Te_3 specimen.

At present stage, we are estimating the structure factor $S(Q)$ of the amorphous As_2Te_3 by applying the numerous corrections to the observed intensity.

[1] . T.Miyanaga, H.Hoshino, H.Ikemoto, M.Yuza, I.Yamamoto and H.Endo, J. Phys. IV 7 (1997) C2-1001.
[2]. H.Hoshino, I.Yamamoto, T.Miyanaga, H.Ikemoto and H.Endo, J. Non-Cryst. Solids (in press).