Structural Phase Transition of Molecular Solids under High Pressure

***Haruki Kawamura (1227), Naoki Matsui (3462), Isao Nakahata (3463), Kazutaka Nakano, Toshiki Nakano and Yuichi Akahama (1226)**

Faculty of Science, Himeji Institute of Technology, Kanaji, Kamigohri, Hyogo 678-12

Introduction

Molecular solids are constructed by two types of chemical bonds, intermolecular bonds and intramolecular bonds. As the intermolecular bonds in a molecular solid generally are much weaker than the intramolecular bonds, the application of pressure has greater effect on the intermolecular bonds, and hence it leads to a structural phase transition and/or rearrangement of chemical bonds through the tuning of the intermolecular interaction.

In this report, we present pressure-induced structural phase transitions of carbon tetrachloride and rhombohedral selenium consisting of Se_6 molecules.

Experimental

A diamond anvil cell was used for high-pressure generation. High-pressure x-ray diffraction experiments were carried out by an angle-dispersive method by the use of an image plate detector. The synchrotron radiation was monochromatized to the wavelength of 0.453 Å by the Si(111) double monochromator.

Results

Figure 1 shows the diffraction pattern of the IV phase of CCl_4 at 2.46 GPa. It is assigned to a cubic Pa3 structure with a lattice constant of 9.423 Å. In the figure, R denotes the diffraction lines from a ruby chip used as a pressure indicator.

Figure 2 shows the diffraction profiles for rhombohedral selenium consisting of Se_6 molecules under various pressure. A successive phase transformation is observed to occur in two stages under high pressure. The first is from the rhombohedral to the trigonal phase which is a stable form of selenium consisting of polymeric chain molecules at ambient pressure. The second stage of transition starts at the pressure of around 16 GPa. This structural phase transformation accompanies metallization.

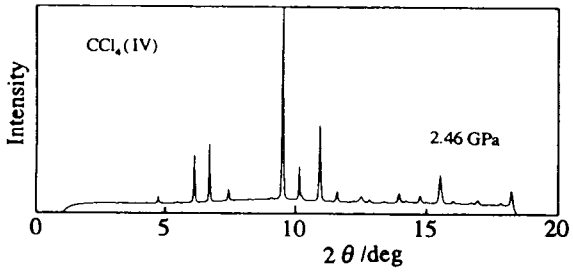

Figure 1 X-ray diffraction pattern of CCl_4.

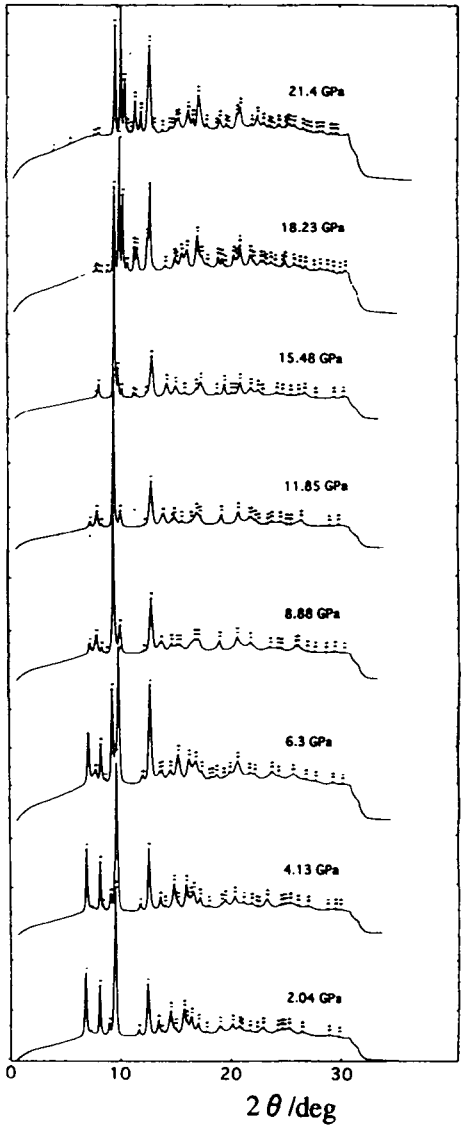

Figure 2 X-ray diffraction profiles for Se_6 under various pressures.