Structural Phase Transition of Molecular Solids under High Pressure

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Introduction

Since molecular crystals are crystallized by weak van der Waals force, many phases are produced through the different orientational arrangements of molecules in the crystal. Figure 1 shows the proposed phase diagram of CH_4 at present. In this diagram, only phase I and II have been crystallographically disclosed, while other phases have been determined through spectroscopic analysis. Under isothermal compression of room temperature methane crystallizes into a fcc structure (phase I) at about 1.2 GPa. It succesively transforms into phase A and phase B.

In this report, we present the results of powder x-ray diffraction analysis of phase A.

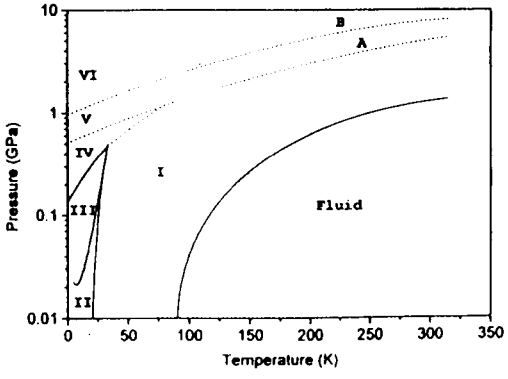

Figure 1 Proposed phase diagram of methane.

Experimental

Powder x-ray diffraction experiments at high pressure and room temperature were carried out by the angle dispersive method using a diamond anvil cell (DAC) and an image-plate detector. Liquefied CH_4 and a ruby chip were loaded into a small hole of the metal gasket (U-700) in the liquid nitrogen cooled DAC. Pressure was determined by the ruby fluorescence method. The synchrotron radiation was monochromatized to the wavelength of 0.4528 Å by the Si (111) double monochromator.

Results

Figure 2 shows the diffraction pattern of phase A of solid methane at pressure of 7.0 GPa. The pattern is assigned to a rhombohedral lattice with lattice parameters of aH=8.637 Å and α =89.37° , which is isostructure of phase I of CF_4 and phase Ib of CCl_4. The result suggests that the molecules still rotatein phase A.

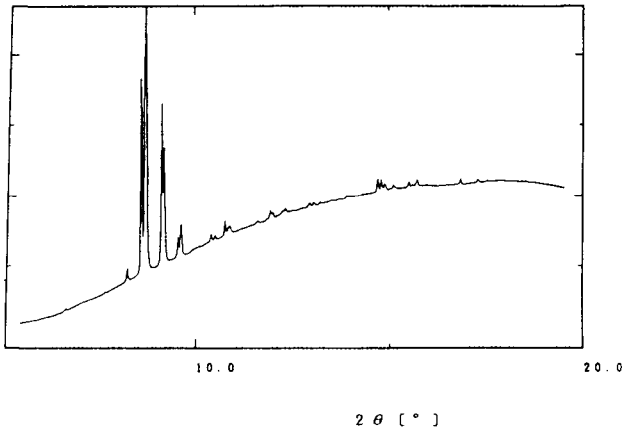

Figure 2 X-ray diffraction pattern of solid methane at 7.0 GPa.