Structural Studies of NbI_4 under High Pressure

***Haruki Kawamura(1227), Isao Nakahata(3463), Naoki Matsui(3462), Kazutaka Nakano(3492) and Yuichi Akahama(1226)**

Faculty of Science, Himeji Institute of Technology, Kanaji, Kamigohri, Hyogo 678-1297

Introduction

Niobium tetraiodide, NbI_4, is a quasi one-dimensional semiconductor at atmospheric pressure. NbI_4 crystalizes in the orthorhombic space group $Cmc2_1$ at ambient conditions.The structure of NbI_4 is based on a distorted hexagonal close-packing of the iodine atoms. One-fourth of the available octahedral holes are occupied by niobium atoms to give infinite linear chains formed by NbI_6 octahedra sharing opposite edges.

A pressure-induced insulator to metal transition has been reported that the electrical resistance and the activation energy decrease continuously with increasing pressure and the activation energy goes to zero at pressure around 15 GPa.

In this paper, we report the results of powder x-ray diffraction experiments for NbI_4 at pressures up to 19 GPa.

Experimental Procedure

Powder x-ray diffraction experiments at high pressure and room temperature were carried out by the angle dispersive method by the use of a diamond anvil cell (DAC) and an image-plate detector. Since the compound is extremely sensitive to water and oxygen, it was ground into fine powder in the dry box filled with nitrogen gas and loaded with a ruby chip into a 0.3 mm diameter hole of a metal gasket (U-700). No pressure transmitting medium was used because of the compound being dissolved in alcohol. Pressure was determined by the ruby fluorescence method.

Results

Figure 1 shows the typical diffraction patterns of NbI_4 at various presures. The diffraction pattern at 1.0 GPa depicted in the lowest pannel was assigned to the orthorhombic lattice with the space group of $Cmc2_1$. With increasing pressure, the pattern did not appreciably change without the smearing out of some diffraction peaks due to the increasing of peak width. The d values of all lines exhibit smooth changes and the relative intensities of reflections remain almost constant up to 19 GPa. The intensities of diffraction peaks on the lower angle side of 004 peak, however, gradually decreased with increasing pressure. These results indicate that the orthorhombic lattice is still retained at pressures up to 19 GPa. These results indicated that the metallization was not accompanied by the structural phase transition. The arrangement of the iodine atoms, however, came closer to an hcp at the higher pressures.

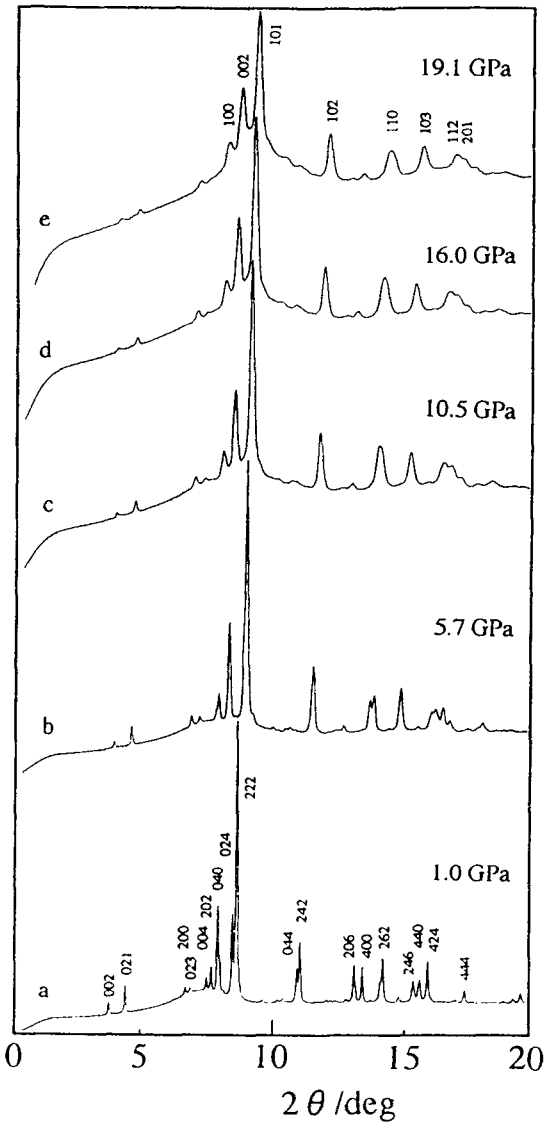

Fig. 1 Typical difraction patterns of NbI_4 at various pressures