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Electron density Analysis of hexamethylenetetramine under high pressure

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Hexamethylenetetramine (HMT; $C_6N_4H_{12}$) is well known as a simple organic compound that has very high symmetric crystal structure (cubic, $I\bar{4}3m$). In previous study, the electron density distributions of HMT at R.T. and 18K were analyzed by the Maximum Entropy Method (MEM). In this study, the electron densities of HMT under high pressure were obtained by MEM using Synchrotron Radiation powder data.

The high pressure X-ray diffraction experiments were performed at SPring-8 BL10XU using diamond anvil cell (DAC) at R.T. The wavelength of X-ray was 0.496Å. The powdered samples were loaded into a hole of Rhenium gasket with small ruby crystals. The diameter of the flat parts of diamonds was 0.45mm. As pressure transmitting medium Helium was used. The diffraction data were obtained at 0.7, 1.4, and 3.4GPa. Each exposure time of X-ray were 40 minutes. In order to compare with previous data, the diffraction experiment without DAC (0.0GPa) was also performed.

There were no significant differences among obtained four diffraction pattern. The crystal structure of ambient pressure was maintained up to 3.4GPa. The MEM/Rietveld analysis was performed for obtaining electron densities. Observed and calculated data showed good fitting in all data. Reliable factors of Rietveld analysis were R_I=2.4, 3.2, 2.5, and 3.0% for 0.0, 0.7, 1.4, and 3.4GPa, respectively. The minimum d-spacing for all data was 1.0Å.

The lattice constant of 3.4GPa was smaller than that of 0.0GPa 6%. However, the bond length between C and N of 3.4GPa was smaller than that of 0.0GPa only 0.7%. This suggested that the region of inter molecule was compressed with the form of molecule maintained. It was also found that the temperature factors for all atoms had a tendency to decrease as the pressure rises.

Fig.1 shows MEM electron densities of HMT (110) plane at 0.0 and 3.4GPa. In Fig.1(b) it can be seen electrons of hydrogen atom as lobes which is shown by arrows. On the other hand, lobes can be hardly seen in Fig.1(a). Fig. 1(b) is similar to MEM densities at 18K. Therefore, it is considered that changes of electron densities by high pressure are close to changes by low temperature in this pressure region.

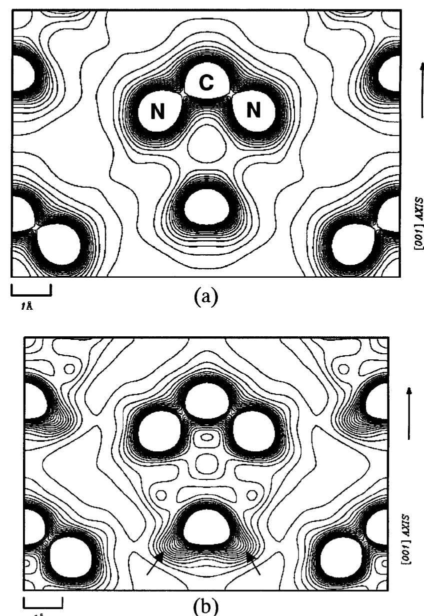

Fig.1 MEM densities of HMT (110) plane at (a) 0.0GPa and (b) 3.4GPa. Contour lines are drawn from 0.1 to 2.1 with 0.1[e/Å^3] step width.

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SCM-XAFS: Selective observation of surface traps in the ~nm region

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In quantum structures, even one-atomic-scale electron traps, such as local distortions and point defects, modify the quantum state. In order to achieve the well-defined quantum structures, the selective analysis of trap centers in selectable ~nm regions is necessary. In recent years, the capacitance XAFS method, in which the absorption spectrum is measured by the x-ray photon energy dependence of the capacitance involved in a diode structure, was proposed[1,2]. In this study, XAFS measurements using a scanning capacitance microscope (SCM-XAFS method) are performed. Though the concept of this method is the same as the capacitance XAFS method, trap centers in selectable ~nm regions would be analyzed by using a scanning probe.

An Au-coated Si cantilever is adopted for capacitance detection at a selectable local area. The point contact of the tip with a semiconductor surface locally makes a metal-oxide-semiconductor (MOS) diode structure owing to a native oxide. The x-ray irradiated into this MOS diode induces a photoemission of localized electron in the trap center, resulting in capacitance changes. The sample is Sn-doped (100) oriented GaAs (GaAs:Sn). The Sn density is 1×10^{17} /cm^3. According to the dangling bonds on the surface, the electrons are localized at many kinds of trap centers.

Figure 1 indicates the x-ray photon energy dependence of the capacitance signal intensity, i.e., SCM-XAFS spectra. In this experiment, applied bias V_b is varied from -0.4 V to +0.4 V. We can clearly observe the edge-jump at the Ga K-edge (10.375 keV) and a number of resonant peaks; ***XAFS spectrum in local region can be obtained by this method.*** Moreover, strong V_b dependences are found in the resonant peaks denoted by P_1~P_5, e.g., the P_4 and P_5 are resonantly observed at V_b = -0.4 V and +0.2 V, respectively. This result suggests that ***trap center selection can be achieved by V_b control.*** The trap selection mechanism can be explained as follows.

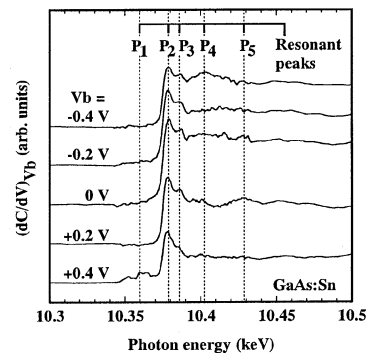

Fig. 1 SCM-XAFS spectra at the Ga K-edge.

Figure 2 shows band diagrams of SCM-XAFS for (a) V_b = -0.4 V and (b) +0.2 V. In this figure, only the origins of P_4 and P_5 are discussed for simple explanation. However, similar models are available for the other resonant peaks. The GaAs:Sn surface is considered to have at least two kinds of surface electron traps, traps 1 and 2, which have energy levels L_{trap1} and L_{trap2}, respectively, in the GaAs band gap. As shown in Fig. 2(a), assuming that the Fermi level in the semiconductor E_f corresponds to L_{trap1} at V_b = -0.4 V, the SCM-XAFS measurement is sensitive to trap 1, because L_{trap2} above E_f has no localized electron. On the other hand, when V_b = +0.2 V, E_f is equal to L_{trap2} as shown in Fig. 2(b). In this case, since the localized electron always occupies L_{trap1} below E_f, the SCM-XAFS signal emphasizes the absorption signal related to trap 2. Therefore, the trap selection by V_b control is realized, and P_4 and P_5 in Fig. 2 can be attributed to traps 1 and 2, respectively.

References

1) M. Ishii *et. al.*: Appl. Phys. Lett. **74** (1999) 2672.

2) M. Ishii, Phys. Rev. B **65** (2002) 085310.

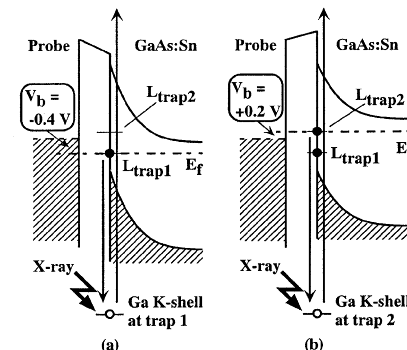

Fig. 2 Band diagram of SCM-XAFS for (a) V_b = -0.4 V and (b) +0.2 V.