10A/2007G020

X-ray thermal diffuse scattering study of CdTe to examine elastic constants under high pressure

Daisuke OHTSU[1], Maki OKUBE[1], Takahiro KURIBAYASHI[2], Yasuhiro KUDOH[2], Akiko NAKAO[3], Satoshi SASAKI*[1]
[1]Materials and Structures Lab., Tokyo Inst. Tech., Nagatsuta, Yokohama 226-0803, Japan
[2]Inst. Mineral. Petrol. Econ. Geol., Tohoku University, Sendai, 980-8578, Japan
[3] Photon Factory, KEK, Tsukuba 305-0801, Japan

Introduction

Cadmium telluride CdTe is the II-VI semiconductor and has attracted to various applications to optoelectronic devices. CdTe has the zinc-blende structure at ambient pressure and transforms to the intermediate cinnabar phase in a pressure range of about 2.5 to 4 GPa, before reaching the rock-salt structure. An accurate description of the elastic property for CdTe is important because it provides a link between the mechanical and dynamical behaviours of crystals in concerning the nature of phase transition.

The elastic constants can be related to the X-ray intensity of thermal diffuse scattering (TDS), which arises from the scattering of the incident beam by phonons. The TDS approach is useful even for a small and opaque crystal loaded in a diamond-anvil cell (DAC). In this study, the pressure dependence of the elastic constant of CdTe is investigated on the basis of the observation of TDS.

Experimental

At each experiment, a single crystal of CdTe was loaded in a modified Merrill-Bassett-type DAC with a gasket made from stainless steel. The pressure was measured using the ruby-fluorescence method. Only zinc-blende phase was investigated in the pressure range close to the phase boundary. The TDS intensity was measured with a vertical-type four-circle diffractometer at the BL-10A of Photon Factory. A wavelength of λ = 0.7 Å was selected by a Si(111) monochromator. The TDS intensities were measured in two-dimensional reciprocal area with two of [100], [010] and [001] passing through 004, 220 and 111 reciprocal lattice points at room temperature.

Results and discussion

The phase-transition pressure was determined to be P = 3.79 GPa from the observation of the intensity variation for 004 Bragg reflection.

Figure 1 shows observed contours of equal intensity of CdTe on the [010] projection, measured at each point of the reciprocal grids around the 004 Bragg peak at P = 0.27 GPa in the DAC. The TDS of X-rays is caused by the lattice vibration. The directions of vertical and horizontal axes are [001] and [100], which are related to longitudinal and transverse waves of velocity, respectively. The shape of curves of isodiffusion surrounding the Bragg peak was obtained from the diffuse intensity, which was compared with the calculated isodiffusion surface (Fig. 1b) [1].

The ratios of elastic constants were examined changing the pressure. The pressure dependence c_{11} of CdTe coincides with the result of the first-principle calculation [2]. The ratios of c_{11}/c_{44} and c_{11}/c_{12} were also determined as a function of pressure.

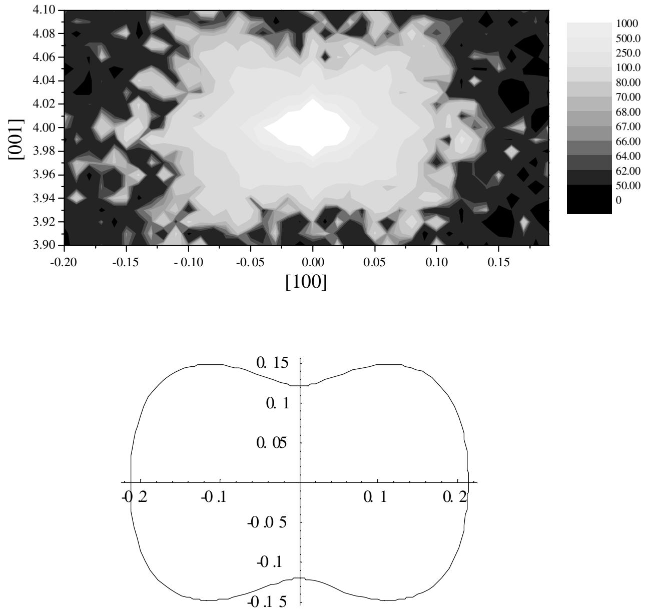

Fig. 1: (a) X-ray intensity distribution around the 004 Bragg peak of CdTe at P = 0.27 GPa. (b) Isodiffusion surface of TDS around 004 calculated from the elastic constants of CdTe; Horizontal [100], vertical [001].

References

[1] H. A. Jahn, Proc. Roy. Soc. A, 179, 320 (1942).
[2] E. Deligoz et al., Physica B, 373, 124 (2006).

* sasaki@n.cc.titech.ac.jp