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Thermal expansion of 4H-SiC

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Introduction

Lattice constants are basic parameters specific for each material, and they vary depending on temperature. It is important to know their behaviors at high temperature in order to control crystal growth and device fabrication. Silicon carbide (SiC) is a wide-gap semiconductor and it has been extensively studied for developing high-efficiency power-electronic devices. Thermal information of this material is especially important because the crystal growth needs high temperatures, such as over 2500 K and 1700 K for bulk crystal and epitaxial film growths, respectively. In this study, we have performed precision measurements of lattice constants of SiC at high temperature up to 1600 K, and thermal expansion coefficients were obtained as a function of temperature.

Experiment and Results

In order to determine the lattice constants with high precision, special attentions were paid to 1) quality of specimen, 2) measurements of angle, and 3) control and measurement of specimen temperature.

Commercially available SiC wafers contain significant lattice distortions with high density of dislocations. The measured Bragg angles, therefore, show position dependence in a wafer, and the accuracy in the lattice constants was limited to the order of 10^{-2} nm. The accuracy was significantly improved by using high-quality wafers as a specimen, and the degree of accuracy was improved by 2-3 digits. The specimen was a 4H-SiC wafer grown with the RAF process [1], of which surface orientation was 4°-off (0001).

X-ray diffraction measurements were performed at beamline BL14B. X-ray of wavelength 0.066 nm was tuned with a Si 440 triple monochromator. The wavelength was determined by measuring the lattice constant of Si using $\bar{3}33$ and $51\bar{1}$ reflections.

Rotation angle of specimen was evaluated with a rotary encoder, but true angle can deviate from the displayed value due to torques induced by electric cables and water tubes equipped to the furnace. To suppress the accidental errors of this kind, we selected sets of diffraction planes to reduce the total rotation angle for the measurements. In order to determine the lattice constants a and c of the hexagonal cell, two pairs of diffraction planes, $\bar{2}022$, $20\bar{2}2$ and $\bar{3}034$, $30\bar{3}4$, were selected. These settings needed the rotation of as small as 7.4° at most. A series of measurements for these diffractions were repeatedly performed at each temperature with about 100 K interval.

Specimen was set at the center of the furnace with N_2 gas atmosphere for high temperature measurement. The specimen was covered with BN walls to block direct radiation from the carbon heaters. Two sets of Pt-PtRh thermocouples were used for measurement of specimen temperature and control of heater current. The specimen temperature was calibrated using the lattice constant of Si based on a standard data given by Okada and Tokumaru [2]. The lattice constants, a and c, were obtained in the temperature range from room temperature to 1700 K during both heating and cooling processes. The lattice constants were obtained with accuracy of 6 significant digits. The temperature dependence of the unit cell volume is shown in Fig. 1.

Thermal expansion coefficients α_a and α_c for the a and c axes were defined by rate of temperature variance of the lattice constants as $\alpha_a \Delta T = \Delta a / a$ and $\alpha_c \Delta T = \Delta c / c$, and in conclusion, they were determined in the form,

$$\alpha(T) = C_1\{1 - \exp[-C_2(T - C_3)]\} + C_4,$$

by fitting C_i (i=1,…,4) to the experimental data.

Acknowledgment

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References

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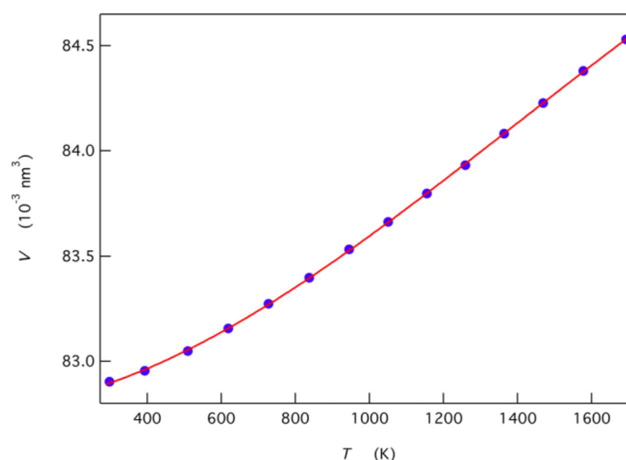

Fig. 1 Temperature dependence of unit cell volume of 4H-SiC.