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Temperature Variations of Lattice Constants for Trigonal Tellurium

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1 Introduction

Trigonal tellurium (t-Te) has a chain structure with two-fold coordinated covalent bonds. The lone-pair orbitals overlap with the antibonding orbitals in adjacent chain. The overlapping between lone-pair and antibonding orbitals in adjacent chain brings about interchain interactions and forms the trigonal structure. The overlapping weakens the covalent bonds and elongates the length of covalent bonds. Tellurium is a characteristic element, because it has a hierarchic structure.

Selenium which is congener element with tellurium has a unique temperature variations of lattice constants[1]. While the lattice constant of a-axis increases with temperature, the lattice constant of c-axis is nearly constant. We report the temperature variations of the lattice constants of t-Te in this report.

2 Experiment

A bulk of t-Te was crashed in argon gas circumstance for preventing oxidization. The powder was filled in the glass capillary with a diameter of 0.3 mm. The X-ray diffraction (XRD) measurements were done at BL19B2 of SPring-8 as Priority Program for Disaster-Affected Quantum Beam Facilities. The X-ray energy used for the XRD measurements was 12.40keV. The lattice parameters were obtained by using CellCalc[2].

3 Results and Discussion

Figure 1 shows the temperature variations of the lattice constant of a-axis. The length monotonically increases with the temperature as other materials. Figure 2 shows the temperature variations of the lattice constant of c-axis. The length of c-axis slightly decreases with temperature, which is different from other materials. In the case of t-Se the lattice constant of c-axis is nearly constant.

These results implies that the thermal expansion of t-Te is attributed to the elongation of a-axis. The length of a-axis is close relation with the interchain interactions, while that of c-axis is related to the chain which is a primary structure. The interchain interactions are influenced more than that of the intrachain interactions by the temperature. The expansion of the distance of the inter chains brings about the decreasing of the overlapping between the LP and anti bonding orbitals. The decrease induces the strengthening of the covalent bond, which causes the shortening of the lattice parameter of c-axis.

Compared to the case of Se, tendency of the value of a-axis is similar while that of c-axis is different. The interchain interactions of t-Te is stronger than that of t-Se, so the expansion of a-axis induces the strengthening of the covalent bond, which brings about the shortening of c-axis.

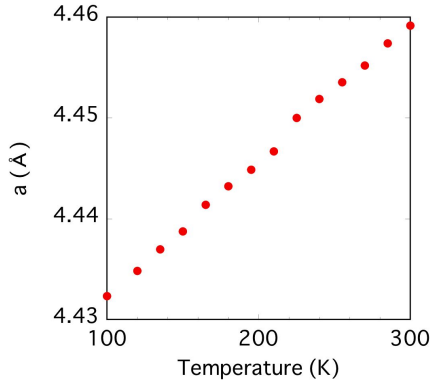

Fig. 1: The lattice constants of a-axis for the trigonal tellurium.

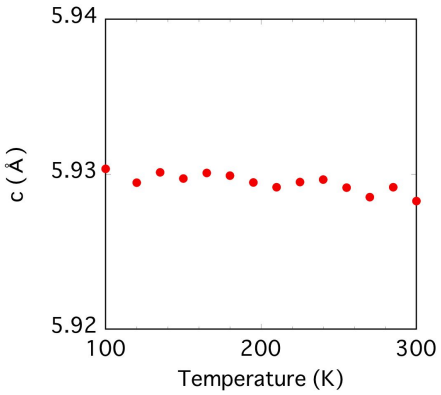

Fig. 2: The lattice constants of c-axis for the trigonal tellurium.

References

[1] Y, H, Zhao, K. Zhang, and K. Lu, Phys. Rev. B, 56 (1997) 14322
[2] http://homepage2.nifty.com/ hsc/soft/cellcalc.html

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