

High pressure phase III of tellurium

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Introduction

Selenium (Se) and tellurium (Te) at ambient condition have trigonal form which consists of 3_1 helix chain molecules. With increasing pressure, both Se and Te change from the molecular crystal, through several high-pressure phases, to bcc metallic phase.^{[1], [2]} In the process of this pressure-induced molecular dissociation, inter- and intramolecular chemical bonding-characters are expected to change with pressure. In order to discuss the pressure dependence of the bonding character in detail, it is necessary to obtain the electron density distribution of Se and Te at various pressures by maximum entropy method (MEM). Since the structure of the high pressure phases of Te-III is ambiguous,^[3] however, the correct structure of Te-III has been obtained before the X-ray structural analysis by the MEM.

Experimental

The powdered samples of commercial tellurium with 99.999% purity were loaded into a diamond-anvil high-pressure cell. Methanol : ethanol : water mixture in 16 : 3 : 1 ratio was used as pressure-transmitting medium. Incident X-ray beam was monochromatized to a wavelength of 0.6200 Å at BL-18C. X-ray diffraction patterns were analyzed using Rietveld refinement program RIETAN-94.^[4]

Results and Discussion

Previously reported phase transitions from Te-I to Te-II, and from Te-II to Te-III are observed at 4 GPa and 7 GPa, respectively.^{[1], [5]} The phase transition from Te-III to Te-IV is observed at 28 GPa. This phase transition is clarified to be of second order, because the X-ray diffraction pattern changes continuously with pressure at pressure between 7 GPa and 32 GPa where the next phase transition from Te-IV to Te-V occurs.

To determine the structure of Te-III, Rietveld analyses were performed using many kinds of unit cells and space groups which were derived from rhombohedral Te-IV lattice. Minimum reliability factor is obtained for a monoclinic lattice whose space group is $C2/m$. The reliability factor (R_{wp}) is less than 15 % for all Rietveld analyses of the high pressure phase at pressure between 7 GPa and 28 GPa. The obtained structure parameters at 10.4 GPa are as follows.

$$\begin{aligned} a &= 8.3790(14) \text{ \AA}, & b &= 4.7300(8) \text{ \AA}, & c &= 3.8710(7) \text{ \AA}, \\ \beta &= 88.63(1)^\circ, & V &= 153.38 \text{ \AA}^3, & Z &= 6, \\ x_1 &= 0 \text{ (fixed)}, & y_1 &= 0 \text{ (fixed)}, & z_1 &= 0 \text{ (fixed)}, \\ x_2 &= 0.328(8), & y_2 &= 0 \text{ (fixed)}, & z_3 &= 0.673(21). \end{aligned}$$

The structure of Te-III is shown in Fig. 1. Solid lines represent the short bonds of about 3 Å. This zigzag layer structure is different from those obtained for tellurium and selenium previously.^{[5], [6]}

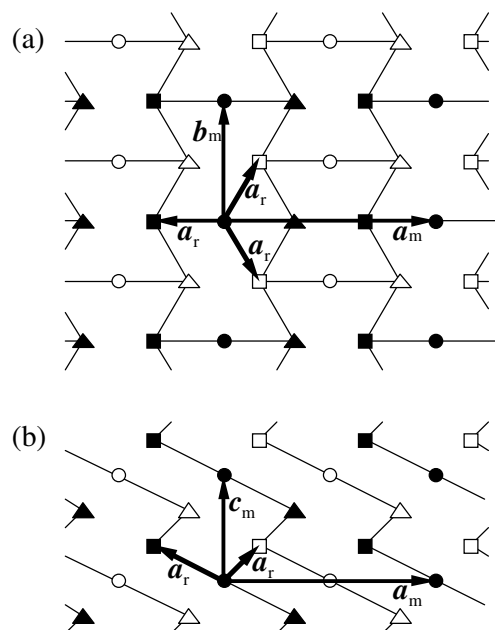


Figure 1. The structure of Te-III phase viewed along the c -axis (a) and the b -axis (b). Solid lines show the short bonds of about 3.0 Å. The symbols a_m , b_m and c_m represent the lattice vectors of Te-III monoclinic phase. The symbol a_r represents the lattice vector of Te-IV rhombohedral phase.

References

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