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Size Dependence of the Lattice Parameters of Tellurium Nanocrystals

Hiroyuki Ikemoto, Akimichi Goyo, Yasuhiro Okuda, and Hitoshi Maekawa
Faculty of Science, University of Toyama, Gofuku 3190, Toyama 930-8555, Japan

Introduction

Trigonal tellurium (t-Te) has a chain structure with two-fold coordinated covalent bonds. The hybridization between lone-pair orbital and antibonding orbital in adjacent chain brings about interchain interactions which affect intrachain covalent bonds. We have reported the structural parameters obtained by EXAFS analysis of the Te nanoparticles [1][2].

The nanoparticles are composed of a mixture of crystalline and amorphous phase. We report the size dependence of the lattice parameters of the Te nanocrystals.

Experimental

Layers of Te and NaCl were deposited alternately onto alumina substrates from alumina crucibles. The thin Te films were discontinuous with isolated island formation, so a sample of Te nanoparticles isolated in NaCl matrix was obtained. The size of the islands was controlled by the change of the thickness film, which was monitored with a quartz oscillator. The ratio of the film thickness between Te and NaCl is 1:20 for all samples. Samples are represented by their average thickness of the Te thin films in this report.

The X-ray diffraction (XRD) measurements were done at BL8B of the Photon Factory in KEK. The X-ray energy used for the XRD measurements was 12.40keV. The XRD measurements were carried out at room temperature. The lattice parameters were obtained by using CellCalc[3].

Results and Discussion

XRD patterns for the Te nanoparticles are shown in Fig. 1. All Bragg peaks are assigned to t-Te and NaCl, and peaks of oxide and chrolide of Te are not observed.

Measured lattice parameters (a and c) of the Te nanocrystals with different film thickness are shown in Fig. 2. The Te nanocrytalals with thickness thinner than 5 nm have values of a evidently above the crystal lattice parameter a_0 (=4.456 A), while the Te nanocrystals with thicker film thickness have values of a approximately equal to a_0. The value of a is found to increase significantly with a reduction of crystalline size. Meanwhile, the values of c monotonically decrease from the crystal lattice parameter c_0 (=5.921 A) with a decrease in the film thickness. The opposite size dependence of the lattice parameters is characteristic of the hierarchic elements. Compared to the case of Se that is congener of Te, tendency of the value of a is similar while the value of c is quite different with that of the Se nanocrystals[4]. The interchain interactions of Te is stronger than that of Se, so the expansion of a-axis induces the strengthening of the covalent bond, which brings about the shortening of c-axis.

References

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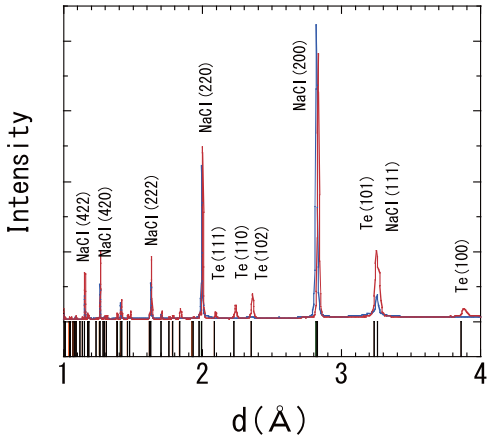

Fig. 1 XRD patterns for the 0.5- and 100-nm-thick films. The red and blue lines denote the XRD spectrum from the 0.5- and 100-nm-thick films, respectively. The vertical bars below zero denote the position of the Bragg peaks from the PDF cards for t-Te and NaCl.

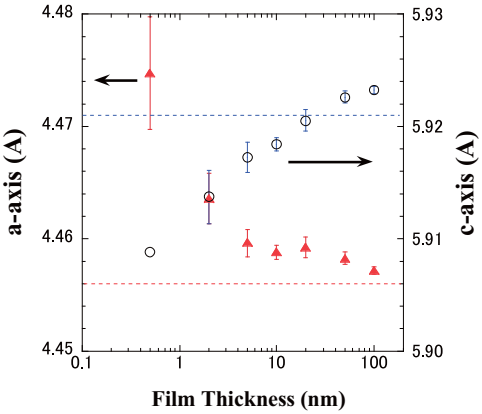

Fig. 2 The lattice constants of the Te nanoparticles. Red triangles and black circles denote the lattice constants of the a-axis and the c-axis,respectively.

* ikemoto@sci.u-toyama.ac.jp