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EXAFS study of amorphous tellurium

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1 Introduction

Tellurium is unique elements that is characterized by hierarchical structures. In trigonal Te (t-Te), the primary structure comprises infinite length chains consisting of covalently bonded atoms. In t-Te, the intrachain first nearest neighbor (1NN) distance (r_{intra}) is 2.835 Å, and the interchain 1NN distance (r_{inter}) is 3.495 Å [1]. The chains are bound by overlapping electronic orbitals between the lone-pair and antibonding orbitals on adjacent chains, which brings about the elongation of the covalent bond.

We have investigated the local structure of the tellurium nanoparticles (n-Te) by EXAFS and the X-ray diffraction. The fraction of the amorphous-like phase increases as the size of n-Te decreases. Information on the local structure of a-Te is useful for understanding that of n-Te.

We report the local structure of a-Te based on the EXAFS results, and we focus on the relation between the intra- and interchain interactions.

2 Experiment

We measured two types of Te films: The first was deposited on a substrate maintained at room temperature, whereas the second was deposited on a substrate maintained at LN_2 temperature. The Te film deposited at room temperature is trigonal (t-Te), whereas that deposited at LN_2 temperature is amorphous (a-Te).

X-ray absorption measurements were performed at NW10A of PF-AR. EXAFS data for the Te K-edge were obtained in fluorescence mode. The measurements were performed at LN_2 temperature. Phase shift, backscattering amplitude and electron mean free path were calculated with the FEFF8 code.

3 Results and Discussion

Distinct EXAFS oscillations of a-Te and t-Te as a function of k are observed up to 16.0 Å^{-1}. While the amplitudes for a-Te and t-Te are similar, the period of oscillation for a-Te is slightly longer than that for t-Te.

Figure 2 shows the Fourie transform (FT) of $k\chi(k)$ for a-Te and t-Te as a function of the radial distance. There are three prominent peaks at 2.88, 3.54, and 4.53 Å for t-Te. The first and second peaks are assigned to the intra- and interchain 1NN correlations, respectively.

The first and second peaks are reserved even in the FT of a-Te. The intensity of the first peak of the FT for a-Te is comparable with that for t-Te, whereas the second peak for a-Te is rather small compared with that of t-Te. The peak position of the intrachain 1NN for a-Te shifts to shorter side than that for t-Te, suggesting that in a-Te, the chain structures are preserved, but the interchain interactions weaken.

For pricise investigation of the intra- and interchain 1NNs, least-squares fitting was applied to the Fourier-filtered $k^2\chi(k)$. Table 1 shows the atomic distance and the coordination number of 1NN. The intrachain 1NN atomic distance for a-Te is 2.77 Å, which is 0.06 Å shorter than that for t-Te. The small values of the covalent bond length and DW imply that the covalent bond strengthens in a-Te. The intrachain 1NN coordination number is 1.97 ± 0.20, which is same as that for t-Te within experimental error.

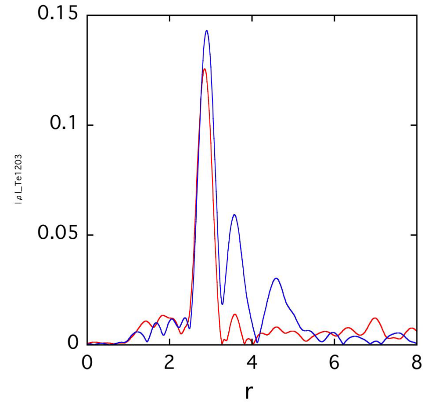

Fig. 1: Fourier transform magnitude of the EXAFS $k\chi(k)$ data for t-Te (blue dotted line) and a-Te (red solid line).

Table 1: Structural parameters obtained from the fit to the experimental EXAFS spectra for a-Te and t-Te.

	r_{intra}(Å)	N_{intra}	DW_{intra} [Å]
t-Te	2.83 ± 0.02	2.00	0.054 ± 0.002
a-Te	2.77 ± 0.02	1.97 ± 0.20	0.049 ± 0.002

[1] Adenis, C., Langer, V. and Lindqvist, O. (1989). Acta Cryst. C45, 941 942.

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