Materials Science

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EXAFS study of Tellurium nanoparticles

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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 report results of extended x-ray absorption fine structure (EXAFS) of Te nanoparticles to investigate the intra- and inter-chain correlations.

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 changed by controlling the thickness of the films, which was monitored with a quartz oscillator. Samples are represented by their average thickness of the Te thin films in this report. EXAFS measurements were carried out at the NW10A of PF-AR. X-ray absorption spectra were measured for Te K-edge (31.8 keV).

Result and Discussion

The EXAFS functions $k\chi(k)$ at 20K for t-Te, the 300-nm and the 0.5-nm-thick films are shown in Fig.1. The amplitudes and phases of 300-nm-thick films are in good agreement with those of t-Te. Period of the EXAFS oscillations of the 0.5-nm-thick film is longer than those of the others, indicating that atomic distance of the 0.5-nm-thick film is shorter than those of the others.

Fourier transform (FT) of $k\chi(k)$ data gives useful information to identify atomic correlations. The experimental EXAFS signals are Fourier-transformed with a hamming window in the range from 2 to 18 Å^{-1}. FTs at 20K for t-Te, the 300-nm- and the 0.5-nm-thick films are presented in Fig.2. The 0.5-nm-thick film is characterized by the shorter nearest neighbor distance and the reduction of the interchain correlation in comparison with the others.

The Fourier peak was filtered in the range of 2.52 and 3.96 Å, inverse Fourier transformed into k-space again and divided by the same Hamming window function in order to extract the peaks originated by the intra- and interchain first nearest neighbors. The EXAFS function, $k^2\chi(k)$, was fitted by a non-linear least square method to the theoretical function within the frame of two-shells model with Te-Te atomic pairs and up to C_3. Phase shift, backscattering amplitude and electron mean free path were calculated by the FEFF8.4 code [1].

Structural parameters obtained from the fit to the experimental spectra at 20K are shown in Table1. The 0.5-nm-thick film is characterized by the shorter intrachain nearest neighbor distance and the reduction of the interchain coordination number in comparison with the others. Coordination number of the 0.5-nm-thick film is close to that of t-Te, suggesting that the two-fold coordinated chain structure is reserved in the 0.5-nm-thick film.

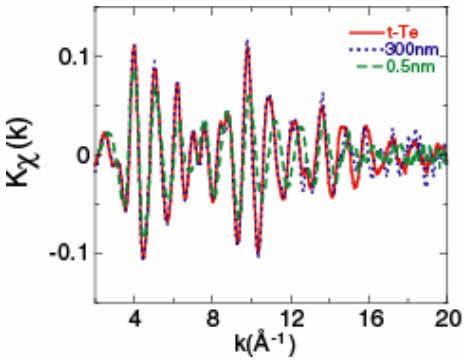

Fig.1: $k\chi(k)$ spectra at 20K for t-Te and the 300-nm- and the 0.5-nm-thick films.

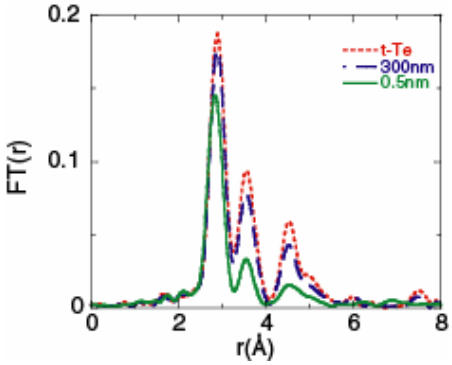

Fig.2: Fourier transforms of $k\chi(k)$ at 20K for t-Te and the 300-nm- and the 0.5-nm-thick films.

Table.1: Structural parameters obtained from the fit to the experimental spectra at 20K for t-Te and the 300-nm- and the 0.5-nm-thick films determined by EXAFS.

	Intrachain			Interchain
	r_1(Å)	N_1	$C_3\times10^{-6}$(Å^{-3})	N_2
[a]t-Te	2.835	2.00		4.00
t-Te	2.836	2.00	-20	4.21
300nm	2.833	2.10	-29	4.30
0.5nm	2.793	1.96	25	1.76

[a]XRD cf. [2]

References

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