Materials Science

NW10A/2007G626

EXAFS study of Tellurium nanoparticles

Akimichi GOYO[1], Shinji YOSHIDA[1], Hiroyuki IKEMOTO[1],
Takafumi MIYANAGA[2] and Kiyofumi NITTA[3]
[1] Univ. of Toyama, Toyama 930-8555, Japan
[2] Hirosaki Univ., Hirosaki 036-8561, Japan
[3] KEK-PF, Ibaragi 305-0801, 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 report the 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 controlled by the change of the thickness film, 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).

Results and Discussion

Table 1 shows structural parameters obtained by the analysis of EXAFS function. Einstein temperatures are derived by an analysis of temperature dependence of Debye-Waller factor. [2]

The coordination numbers of the intrachain first neighbor (1NN) for small particles are close to that of t-Te. This implies that the twofold coordinated chain structure is preserved even in the small samples. The 1NN distances are same as that of t-Te in the thicker samples, but it shortens with decrease of sample thickness below 10-nm-thick films. The bond distance of the 0.5-nm-thick films is 0.042 Å shorter than that of t-Te, and also the Einstein temperature of the 0.5-nm-thick films is higher than that of t-Te. These changes suggest that the covalent bonds strengthen with decreasing of the size for the Te nanoparticles.

The coordination number of the second nearest neighbor (2NN) rapidly decreases below 5-nm-thick films. It reaches about two, which is half of that of t-Te. The reduction suggests that the interchain interactions weaken with decreasing for the size for the Te nanoparticles.

Figure 1 shows the correlation between the 2NN coordination number and the 1NN atomic distances. It is clear that the intrachain covalent bonds strengthen with the loss of the interchain interaction.

Table.1: Structural parameters obtained from the fit to the experimental spectra at the temperature range from 20 to 300K.

	Intrachain			Interchain	
	r_1(Å)	N_1	Einstein Temperature (K)	N_2	Einstein Temperature (K)
*t-Te	2.835	2.00		4.00	
t-Te	2.834	2.05	153	4.23	83
300nm	2.831	2.06	151	4.56	84
50nm	2.830	2.04	152	4.37	80
20nm	2.829	2.03	151	4.31	81
10nm	2.825	2.03	152	4.18	81
5nm	2.823	2.03	150	4.01	80
2nm	2.818	2.01	155	3.82	79
0.5nm	2.788	1.91	170	2.32	71

*XRD cf. [1]

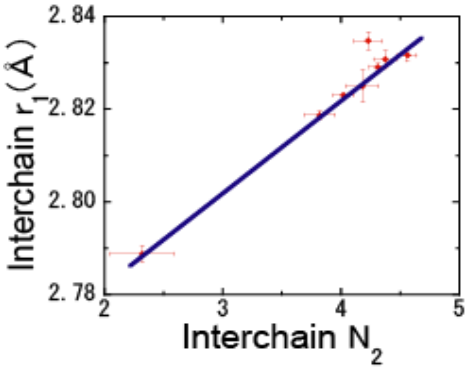

Fig.1: Correlation between interchain coordination number and intrachain atomic distance.

References

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

[2] E.Sevillano, H.Meuth, J.J.Rehr, Phys.Rev.B20.4908 (1979)

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