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Force Constants of Te Nanoparticles

H. Ikemoto[1], A. Goyo[1], H. Maekawa[1], and T. Miyanaga[2]
[1] Faculty of Science, University of Toyama, Gofuku 3190, Toyama 930-8555, Japan
[2]Faculty of Science and Technology, Hirosaki University, Hirosaki 036-8561, 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 most striking results concerning the Te nanoparticles are shrinkage of the covalent bond length and preservation of the coordination number of the covalent bonds within the chains. The twofold-coordinated chain structure specific to t-Te is preserved even in the Te nanoparticles. The bond distance is 0.046 ˚A shorter than that of t-Te, indicating a strengthening of the covalent bonds.

We report the force constans of the Te nanoparticles with two kinds of analyses, that is, the empirical equation of the bond length and the Einstein model.

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

There is an empirical relation between force constant K_B and the covalent bond length R_e:

$$K_B = A \exp(s/R_e) \qquad (1)$$

where R_e is the equilibrium bond length, and A and s are constants throughout a given period in the periodic system[3]. The values of s and A for the fifth period in the periodic are not shown, but the value of s for the third period is close to that for the fourth, and the value of A tends to saturate as the number of the period increases. So we use the values s = 14 [A] and A = 0.53 [N/m] for the fourth period are adopted. Table I shows the force constants obtained by the equation (1). The force constant for the intrachain interactions of the 0.5-nm-thick film estimated from the bond distances is about 1.1 times stronger than that of t-Te.

The harmonic oscillation treatment is another approach to estimating the force constant. The value of the Debye-Waller factors (σ^2) can be expressed by the Einstein model. The Einstein temperature (Θ_E) is obtained from a temperature-dependent study of σ^2. We reported the values of Θ_E for t-Te and Te nanoparticles [1][2]. In the Einstein model, there is the relationship between K_E and Θ_E as follows,

$$K_E = \mu\omega_E^{\,2} = \mu\frac{k_B^{\,2}}{\hbar^2}\Theta_E^{\,2} \qquad (2)$$

where μ is the reduced mass. The force constants calculated by Eq. (2) for t-Te are shown in Table I. The absolute values of the force constants for t-Te do not correspond with those in the literature [4]. Despite this discrepancy, the Einstein model may be used for a rough estimation of the force constants even if this model is very simple. So we apply the relation to the system of Te nanoparticles, and the resulting force constants for the 0.5-nm-thick films are shown in Table I. The relation between K_E and Θ_E shows that the force constant for the intrachain interactions of the 0.5-nm-thick films is 1.3 times stronger than that of t-Te. The two analyses show that the force constants of the covalent bond for the 0.5-nm-thick films is 1.1~1.3 times stronger than that of t-Te.

References

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

TABLE I: Force constants of the intra- and interchain interactions for t-Te and the 0.5-nm-thick films. The force constants K_B and K_E are estimated from the empirical equation for the covalent bond length and the Einstein model, respectively. The values from the literature [4] are also shown.

		K_B	K_E	K[4]
t-Te	Intrachain	74	89	66.4
	Interchain		25	13.3
0.5nm	Intrachain	80	115	
	Interchain		23	