Crystal Structure of $Te_{0.4}Se_{0.6}$

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Introduction

At the atmospheric pressure, the most stable form of selenium and tellurium is trigonal, and they show seversal structural transitions, and semicomductor-to-metal transiton, under pressures. It has been well known that Te-Se mixture also shows interesting electronic properties under high pressure. In the present work we have carried out the structure determination of $Te_{0.4}Se_{0.6}$, of which structure at high pressure can be quenched to the atmospheric circumstance[1], with short wave length of synchrotron radiation.

Experimental

The X-ray diffraction measurements were made on BL-10A beam line at the Photon Factory , KEK. The incident X-ray was tuned at 0.4 Åby 311 diffraction with silicon flat-plate monochromator. One specimen crystal was chosen for intensity measurement after being examined, in particular, in connection with crystalline quality by rotational photography. The size of the specime4n was $230\times130\times150\mu m^3$. The linear absorption coefficient μ=15.76 mm^{-1} thus absorption collection is not required for the present case. The orientation matrix was determined using thirteen strong reflections within $\theta = 15^o$. The lattice constants were determined *a*=8.164, *b*=27.856, *c*=13.852 Å and $\beta = 90^o$. The intensities of the higher harmonics of the monochromated beam were very weak, but further reduced by a discriminator of the detector circuit. The intensity data of the unique region of the reciprocal space were collected in the range $\sin\theta/\lambda \approx 0.5$ by assuming no extinction rule: to collect additional reflections which have non-integer indices due to longer periodicity of the real lattice; namely a×9b×2c , the lattice parameter were defined as *a*=8.164, *b*=250.70, *c*=27.704 Å. 1630 unique diffractions were measured. The integrated intensity was determined by summing up the intensity measured stepwise in the ω scan and subtracting background. After correction for current of synchrotron orbit, a set of structure factor $|F|$ was obtained.

Structure determination and results

According to the observed extinction rule; h0l (l odd), the space group of the material must be Ic or I2/c. For the latter space group, no meaningful result was obtained with small R factor. Thus, we continue the refinement assuming the former space group.

At first, the least-square refinement (SHELX-97 coded by G. M. Sheldric) was carried out assuming monotonic occupancy of 0.4 Te and 0.6 Se atoms at all atomic site. After reaching a minimal R factor of 0.124, the refinement was continued introducing occupation parameter σ of Te fraction at 27 unique sites. Finally we obtained the structure with R=0.098 using isotropic temperature factors. The results of atomic coordinate and occupancy parameter are listed in table.

Table: List of atomic coordinates, isotropic temperature factors and occupation parameters of Te.

site	x	y	z	U_{iso}	σ
1	0	0.0059	0	13×10^{-3}	0.47
2	0.839	-0.0032	0.2022	21	0.10
3	0.110	0.0083	0.3540	19	0.62
4	-0.0139	0.1042	-0.0052	17	0.78
5	0.869	0.1112	0.1962	19	0.10
6	0.1252	0.1272	0.3595	24	0.88
7	-0.0608	0.2166	0.0123	15	0.01
8	0.820	0.2061	0.1639	20	0.64
9	0.095	0.2211	0.3208	11	0.01
10	-0.0354	0.3403	0.0187	12	0.18
11	0.839	0.3315	0.1727	21	0.55
12	0.097	0.3365	0.3341	15	0.01
13	-0.0130	0.4414	0.0070	21	0.99
14	0.843	0.4471	0.2045	20	0.19
15	0.120	0.4341	0.3544	15	0.99
16	0.005	0.4461	0.4975	10	0.01
17	0.835	0.4514	0.6900	28	0.66
18	0.092	0.4443	0.8542	18	0.27
19	-0.0588	0.3269	0.5313	23	0.28
20	0.824	0.3399	0.6819	15	0.74
21	0.104	0.3256	0.8306	16	0.36
22	-0.0602	0.2281	0.5231	22	0.42
23	0.853	0.2179	0.6818	14	0.01
24	0.113	0.2318	0.8366	14	0.87
25	-0.025	0.1151	0.5063	26	0.01
26	0.818	0.0990	0.6794	21	0.69
27	0.085	0.1129	0.8364	13	0.01

References

[1] Y. Ohmasa et al., J. Phy. Soc. Jpn**, 64**, 4766 (1995).

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