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Local Structure Determination of $Te_{0.4}Se_{0.6}$

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Introduction

The crystal structure of $Te_{0.4}Se_{0.6}$ determined by Y. Soejima *et al.* [1] has longer periodic unit cell in a size of $a \times 9b \times 2c$; where the lattice constants *a, b and c* are based on those of the basic structure with space group *Cm* consisting of zig-zag chain of trimer molecule (see Fig.1). In the reference, it is reported that the structure belongs to the space group *Cc* and the lattice constants are a=8.164, b=27.856, c=13.852 Å and β=90˚ at room temperature. As shown in Fig.2, it is also reported that the occupancy of Te atom varies at the unique 27 sites in the unit cell, and

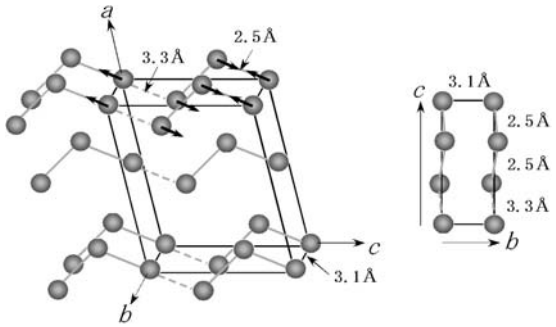

Fig.1 The basic structure of $Te_{0.4}Se_{0.6}$.

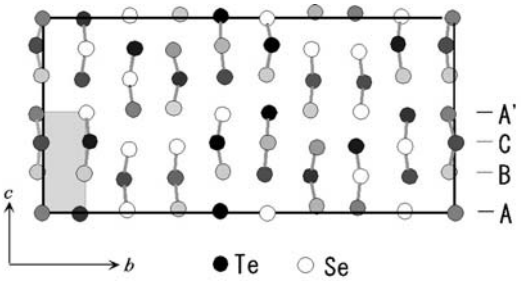

Fig.2 Occupancy of Te atom at 27 unique sites. The shaded part indicates the unit of basic structure shown in Fig.1.

this strongly contributes to the formation of the longer periodic structure. Here we have a question as follow: the variable occupancies of Te atom is the result of the structure determination which introduces an average structure over the area where X-rays are coherent, or the mixture states are realized in the structure. To solve the problem, the local structure determination has carried by using X-ray anomalous dispersion effect of Se.

Experimental

The measurements were made at BL-10A, Photon Factory, KEK. The size of specimen crystal was 230×130×150μm^3. The diffractometer was optimized at 12.44–12.78 keV and intensities of several diffractions which originate in the longer periodic structure were measured as a function of incident energy by a step of 5.5 eV. Observed intensities were corrected for the intensity of incident beam and absorption of the crystal at each energy step, then we obtained structure factor as a function of the incident energy around the absorption edge.

results

In Fig.3, typical examples are shown. The calculated structure factors are in good agreement with those observed. This indicates that the local structure shown in Fig.2 is realized in the structure, and therefore we conclude that the mixture states of Te and Se are specially stable at the sites.

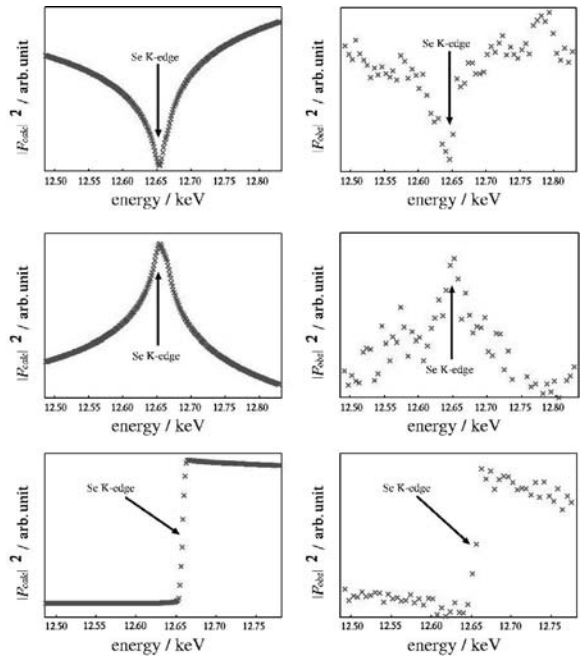

Fig.3 Typical examples of structure factor around Se K absorption edge: top, middle and bottom are 200, 235 and 170 diffraction, respectively. Calculations based on the structure shown in Fig.2 are on the left hand sides, and observed structure factors are on right.

References

[1] Y. Soejima *et al.*, Photon Factory Activity Report, **#18**, 117.

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