Diffuse scattering in α and β Sn Single Crystals

Univ. of Tsukuba Miwako Takahashi

1.Introduction

β-Sn has a body-centered tetragonal structure and is metallic, and transforms to α-Sn at low temperature which is a semiconductor and has a diamond structure. Detailed mechanism of the transformation has been still controversial between diffusive or martensitic. Diffuse scattering in β-Sn has long been studied since 1943[1]. Its intensity distributions show quite characteristic features of asymmetrical and anisotropic shapes in reciprocal space. The origin of the characteristic intensity distributions is regarded to be TDS (Thermal Diffuse Scattering) resulting from lattice dynamics in the β-Sn-structure which belongs to non-symmorphic space group[2]. In our previous neutron-diffraction measurements, it was found that intensity maxima appeared at X-points in the diffuse scattering during the β to α transformation. In order to understand the relation between the diffuse maxima and mechanism of the transformation, energy-resolved diffuse scattering measurements have been performed using a cold-neutron disk chopper spectrometer AMATERAS installed in BL14 at MLF, J-PARC.

2. Experiment

Multiple $E_i$measurements were performed with E_i =4.688, 7.743, 15.17, and 42.10 meV for β-Sn single crystals with two different crystal orientations: hhl and $hk0$ reciprocal planes in the equatorial, at 300K and 230K. Data were analyzed with program *Utsusemi*.

3.Results

Inelastic intensity distributions were compared with diffraction patterns observed in the process of β to α structural transition[3]. Diffuse streaks are observed along $hhl; l = 2n + 1$ with maxima at X-points $hhl; h = (2n + 1)/2$ in the inelastic patterns at $\Delta E > 3$meV at 300K (Fig.1). Quite similar intensity distributions have been observed in the diffraction patterns during β to α transformation (Fig.2). Considering the fact that the intensities of the diffraction patters in Fig.2 include inelastic components around $\Delta E = 0$meV, the X-point-diffuse-maxima observed during the phase transformation can be interpreted as a result of softening of the acoustic modes of transverse phonons at X-points. Several dispersion relations at high-symmetrical reciprocal lines are plotted and compared to the theoretical calculation[2]. The dispersion relations show qualitative agreement between experimental and theoretical results at low energy regions, as shown in Fig.3. Further investigation are necessary for both experimental and theoretical sides to understand the origin of the X-point diffuse maxima from the view point of the softening of the lattice dynamics.

4. Conclusion

Energy-resolved diffuse scattering measurements have been performed for β-Sn single crystals to understand the origin of diffuse maxima observed in the process of β to α transformation. Inelastic intensities at $\Delta E > 3$meV show maxima at the same X-points in the diffuse scattering. The result indicates a strong softening of lattice dynamics has taken place at the X-points during the β to α transformation. Experimental spectra along the high-symmetrical reciprocal lines show qualitative agreement to the calculated dispersion relations.

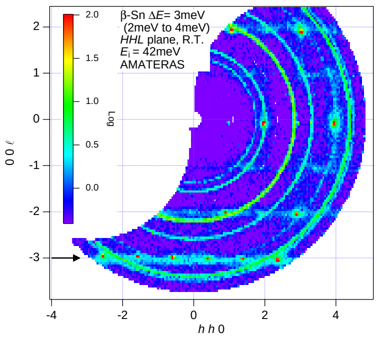

Fig.1 Inelastic intensities of $\Delta E = 3\mathrm{meV}$.

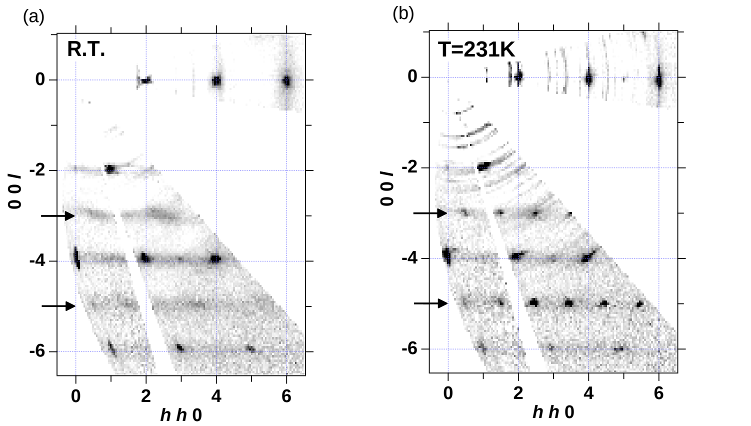

Fig.2 Diffraction pattern at the (a)initial and (b)middle stages of the $\beta - \alpha$ structural transition.

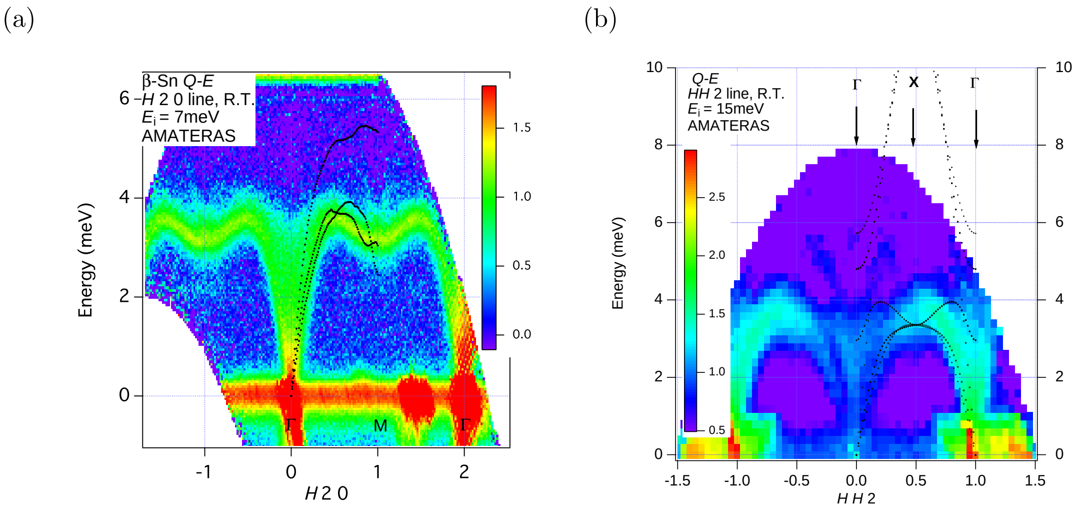

Fig.3 Observed phonon dispersions along (a)$h20$ and (b)$hh2$ reciprocal lines. Black dotted lines represent results of *ab initio* calculation[2].

Reference

[1] J.J. Arlman and R. Kronig; " Investigation of lattice defects by means of X-rays. I. Tin ", Physica, **10**(1943)795.

[2] B.Wehinger, A. Bosak, G. Piccolboni, K. Refson, D. Chernyshov, A. Ivanov, A. Rumiantsev and M. Krisch; " Diffuse scattering in metallic tin polymorphs ", J. Phys. Condens. Matter. **26**(2014)115401.

[3] M. Takahashi, K. Ohshima, and Y. Noda; " Measurement of diffuse scattering in β-tin single crystal ", Nihon Genshiryoku Kenkyu Kaihatsu Kiko JAEA- Review, 2006.