

Abstract No. chri0510

Structural investigation of Zn_4Sb_3 , a promising thermoelectric material

M. Christensen,¹ E. Nishibori,² B. Lundtoft,¹ J. Overgaard,¹ T.R. Jensen,¹ J.-E. Jørgensen,¹ B.B. Iversen,¹

¹ Department of Chemistry, University of Aarhus, DK-8000 Aarhus C, Denmark

² Department of applied Physics, Nagoya University, Nagoya 464-8603, Japan

Beamline(s): X3A1

Introduction: Measurements of the electronic and thermal conductivity have shown that Zn_4Sb_3 fulfils the requirements for a good thermoelectric material. Especially the thermal conductivity approach that expected for amorphous glass and thus Zn_4Sb_3 meets one of the requests for the hypothetical concept of (PGEC) proposed by Slack [1]. The phase diagram of the binary compounds containing Zn and Sb is relatively complicated. Until recently only polycrystalline samples could be produced by quenching the stoichiometrical melt. Lately zone-melting feeding rods of different stoichiometri have been utilised in order to achieve single crystals.

Experiment: High resolution single crystal synchrotron data was obtained at NSLS on beamline X3A1. The data is measured at short wavelength to avoid extinction and thus get data suitable to obtain bonding information through maximum entropy analysis. Measurements were carried out at, room temperature and 15 K. The data collection at the X3A1 beamline at NSLS, greatly improved the characterisation the structure. In the table below the reflections collected at the X3A1 beamline is compared with data collection at a SMART Bruker diffraction equipped with a CCD detector and utilising molybdenum radiation.

	Synchrotron			Molybdenum
	RT before cooling	10 K	RT after cooling	Bruker RT
Total	42740	33501	54746	15688
Unique	5514	5341	5038	1053

The table shows how many reflections it has been possible to measure

Results: From the synchrotron data interstitial sites with low occupancy have been found by inverse Fourier mapping and confirmed by maximum entropy methods. These interstitials may help explain the low thermal conductivity of the material. Heat capacity data, shows a phase transition at about 236 K, which structurally is not fully understood, more investigations are needed to characterise the structure, which is expected to give more clues to the understanding of the low thermal conductivity of Zn_4Sb_3 .

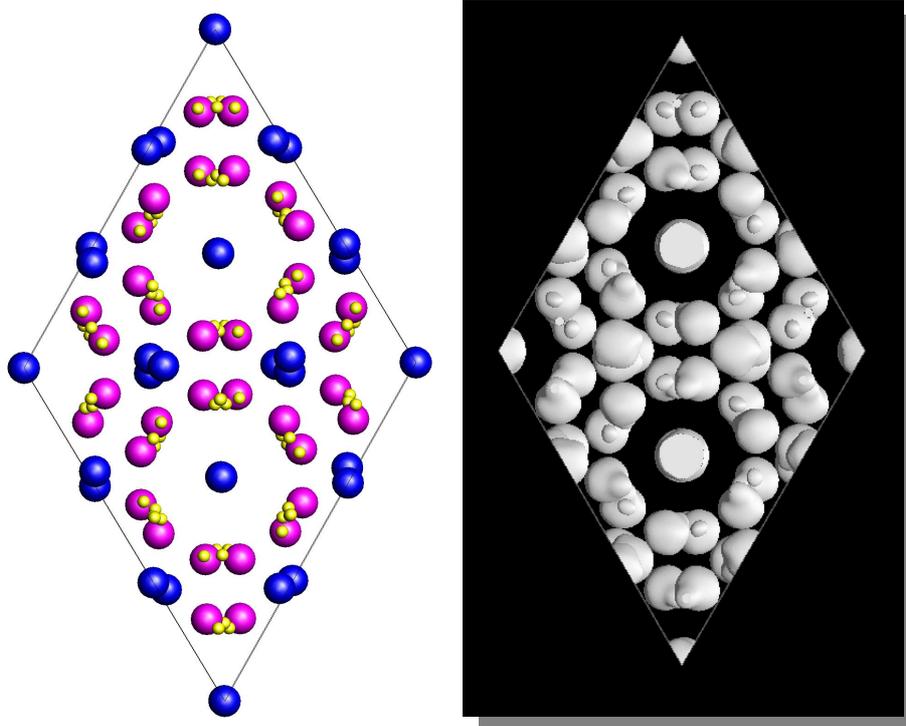


Figure: (left) the structure of Zn_4Sb_3 . (right) Mem density calculation of Zn_4Sb_3 .