ESRF	Experiment title: Temperature dependant total scattering measurements for investigation of atomic and nano-scale structure in thermoelectric Half-Heusler compounds	**Experiment number**: CH-4319
Beamline: ID22	**Date of experiment**: from: 20/06 2015 to: 22/06 2015	**Date of report**: 26/08/2015
Shifts: 6	**Local contact(s)**: Christina Drathen	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Marit Riktor*[1] , Magnus H. Sorby[2], Bjørn C. Hauback[2]

[1] SINTEF, Forskningsveien 1, 0314 Oslo, Norway

[2] Institute for energy technology, PO Box 40, 2027 Kjeller, Norway

Report:

Introduction

The thermoelectric (TE) effect is the direct conversion of temperature differences to electricity and vice versa. Thermoelectricity is currently extensively investigated with the aim to convert waste heat into electricity, but the efficiency is currently too low to be cost-effective in most applications. To increase their efficiency it is necessary to reduce thermal conductivity without significantly disrupting electrical conductivity, i.e. to produce a material with phonon-glass and electron-crystal properties. This can e.g. be done by constructing a crystalline material with point defects and nano-domains, which scatters short and mid-long wavelength phonons, respectively. Furthermore, nano-structuring may change the electronic structure due to quantum confinement or energy filtering, which significantly changes the Seebeck coefficient and the electric conductivity. Knowledge about local structure of bulk material is thus of crucial importance for the understanding and further development of these materials.

Half-Heusler (HH) materials are among the most interesting new candidate materials for thermoelectric applications. They have the general chemical formula *XYZ*, and all three constituent elements can be chosen from a large part of the periodic table, as long as the 8- or 18-electron rule is fulfilled. Adding to the flexibility, it is usually possible to substitute on one or more of the sites to introduce point defects and/or nano-domains. Thermoelectric HH of composition *X*NiSn where *X*=Ti, Zr, Hf is particularly relevant since it is environmentally friendly and has very high thermoelectric performance in the temperature range 400-700 ^{o}C, corresponding to heat sources such as automobile exhaust and industrial waste.

Due to the large flexibility in forming HH compounds, it is often unclear whether some compositions are single-phase solid solutions or consist of different domains. This is important knowledge, since it can guide experiments towards immiscible or miscible systems, depending on which ones perform the best. It is also of high scientific interest to elucidate how local disorder in these compounds can influence their transport properties.

Results

Eight samples of composition *X*NiSb where *X*=Ti, Zr or Hf and mixtures of these were provided by IFE. It has turned out to be very challenging to produce phase pure compounds by arc melting (even after thermal annealing), and all samples were thus measured using the high resolution diffractometer in addition to the temperature dependant scans using the 2D detector. The high resolution data showed that compounds initially believed to be single phase have double peaks (figs 1 & 2). Very good quality data were obtained for all samples, and the work to determine the stoichiometry of the different phases is in progress. Total scattering data will be challenging to analyse due to the phase-coexistence. Thermoelectric measurements on the same samples will be performed, and the results obtained in the present study are expected to contribute with further insight to the atomic and nano-scale structure of the Half-Heusler compounds and to elucidate the correspondence between phase composition, (micro)structure and thermoelectric properties. An article presenting the results from ID22 together with the results from the thermoelectric measurements is planned.

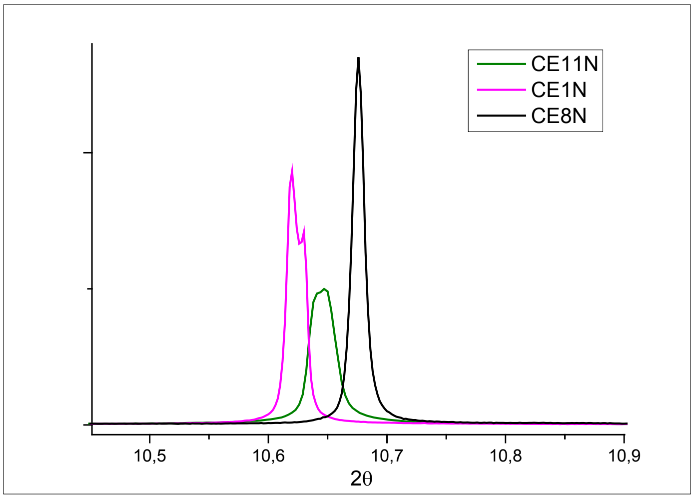

Fig 1. Diffraction data from the high resolution diffractometer show that some of the samples initially believed to be single phase have double peaks, as it is the case of ZrNiSn.

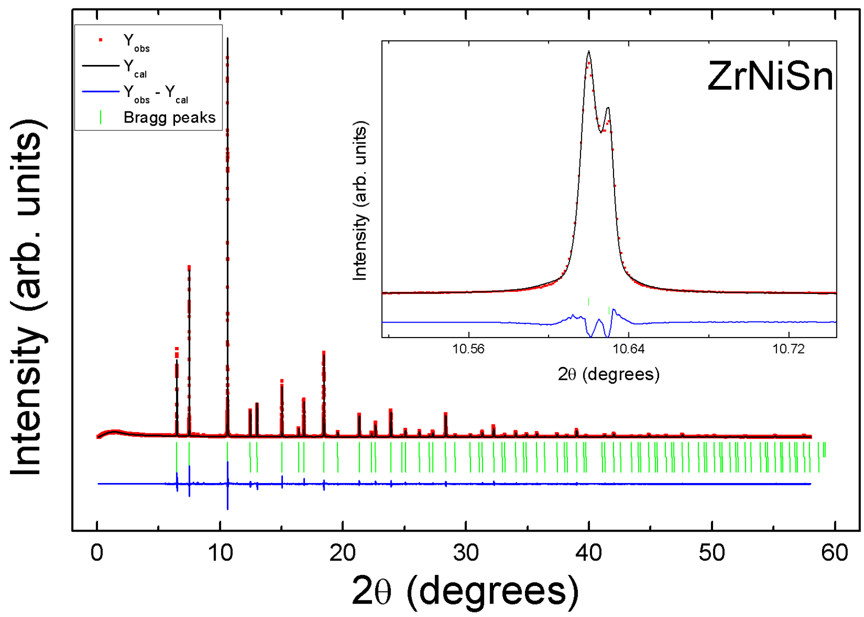

Fig 2. Diffraction data from the high resolution diffractometer of ZrNiSn. Here we can see in more detail the double peak corresponding to a phase coexistance.