Experimental report

16/04/2024

Proposal: EASY-1108 **Council:** 10/2022

Title: Atomic site distributions in TiZnNi2Sb2 half-Heusler thermoelectric

Research area: Materials

This proposal is a new proposal

Main proposer: Jan Willem BOS

Experimental team:

Local contacts: Emmanuelle SUARD

Samples: TiZnNi2Sb2

Instrument	Requested days	Allocated days	From	To
D2B	5	5	25/05/2023	26/05/2023

Abstract:

The aim of the experiment is to determine the distribution of Ti, Zn and Ni over the X (0, 0, 0) and Y (0.25, 0.25, 0.25) sites in the half-Heusler structure [Sb located at (0.5, 0.5, 0.5)], and to check for possible occupancy of a vacant site (0.75, 0.75, 0.75). Neutrons are vital because of the good scattering contrast for these elements (Zn: b = 5.7 fm, Ni: b = 10.3 fm and Ti b = -3.4 fm), which have next to no X-ray contrast. This composition is of interest as a possible thermoelectric with zT = 0.35 at 600 K. The results will go towards a PhD thesis that will be submitted by September 2023.

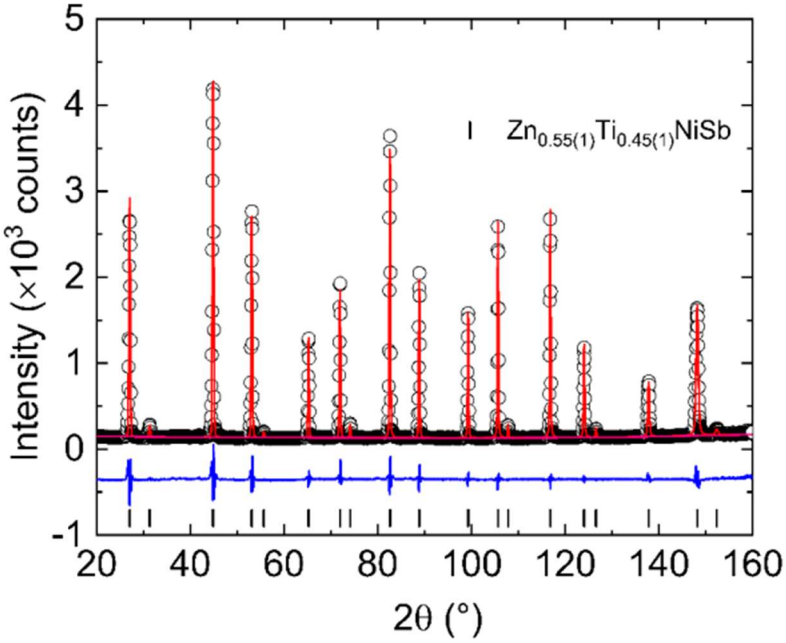
Experimental Report for Proposal EASY – 1108

Proposal Title – Atomic Site Distributions in $TiZnNi_2Sb_2$

This experiment aimed to determine the structure of the novel aliovalent Half-Heusler alloy $Ti_{0.5}Zn_{0.5}NiSb$, which was not possible with X-ray powder diffraction.

An annealed $Ti_{0.5}Zn_{0.5}NiSb$ alloy was pulverized, and data collected on D2B over a period of 4 hours. The dataset collected was of excellent quality, with subsequent Rietveld Refinement allowing confirmation of the half-Heusler structure, with Ti and Zn both occupying the X site in the crystal structure. The quality of the fit can be seen below.

This dataset and the structural information were used in a publication on these materials in the Journal of Materials Chemistry A, with the citation given below.



Rietveld refinement against D2B data for a nominal $Zn_{0.5}Ti_{0.5}NiSb$ sample.

B.F. Kennedy, S.A.J. Kimber, S. Checchia, A.K.M.A. Shawon, A. Zevalkink, E. Suard, J. Buckman and J.-W.G. Bos "Thermoelectric properties of the aliovalent half-Heusler alloy $Zn_{0.5}Ti_{0.5}NiSb$ with intrinsic low thermal conductivity" *Journal of Materials Chemistry* A **11**, 23566 (2023).