Experimental report

17/09/2023

Proposal: 5-23-786 **Council:** 10/2022

Title: Understanding thermoelectric properties in NbCoM0.05Sn (M = Fe, Co, Ni, Cu) half-Heusler compounds by neutron diffraction

Research area: Materials

This proposal is a new proposal

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Samples: NbCo1.05Sn
NbCoSn
NbCoFe0.05Sn
NbCoNi0.05Sn
NbCoCu0.05Sn

Instrument	Requested days	Allocated days	From	To
D2B	3	4	09/06/2023	13/06/2023

Abstract:

Intrinsic interstitial defects are thermodynamically favorable in high-temperature synthesized half-Heusler compounds and manipulate the thermoelectric properties (improving electrical conductivity ¿ & reducing lattice thermal conductivity). They provide a new pathway to boost thermoelectric performance. Here, NbCoSn & NbCoM0.05Sn (M = Fe, Co, Ni, Cu) were synthesized to study the effect of different excessive metals on crystal structure, thermoelectric properties, and to probe correlation between them. The temperature dependence of ¿ in NbCoFe0.05Sn & NbCoCu0.05Sn behave similarly to NbCoSn (semiconductor behavior). In contrast, the electrical transport behavior of NbCo1.05Sn & NbCoNi0.05Sn becomes metallic and increase compared to NbCoSn. Our previous studies show that interstitial defects can modify the electronic band structure in different ways and thus transport behavior. To bridge the correlation between interstitial defects and electrical properties of NbCoM0.05Sn, the site occupation factors of interstitial defects need to be investigated. Since Fe, Co, Ni, Cu have similar atomic form factors, neutron diffraction is highly needed to distinguish them on the 4c and 4d site.

Understanding thermoelectric properties in NbCo$M_{0.05}$Sn (M = Fe, Co, Ni, Cu) half-Heusler compounds by neutron diffraction (5-23-786)

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Four intermetallic half-Heusler NbCo$M_{0.05}$Sn (M = Fe, Co, Ni, Cu) have been prepared and measured at RT first on D2B with an incident wavelength of 1.594 Å. Afterwards the samples are loaded into the furnace and measured at 600 K and 900 K in order to track potential changes on the site occupation of the ideally empty 4*d* position of the crystal structure as well as the elemental distribution between 4*c* and 4*d* site. The samples have been loaded into gold-sealed vanadium cans.

Rietveld refinements in combination with collected high-resolution synchrotron diffraction are currently under way to track the above mentioned changes in the occupation factors.