Experimental report

12/01/2022

Proposal: EASY-724 **Council:** 4/2020

Title: Crystal structures in nanograined-Fe2VAl polycrystals for thermoelectric applications

Research area: Materials

This proposal is a new proposal

Main proposer: Eric ALLENO

Experimental team:

Local contacts: Ines PUENTE ORENCH
Laetitia LAVERSENNE
Vivian NASSIF

Samples: Fe2VAl

Instrument	Requested days	Allocated days	From	To
D1B	14	14	14/02/2021	15/02/2021

Abstract:

Fe2VAl could become a good thermoelectric material if its thermal conductivity could be reduced. This can be achieved by synthesizing Fe2VAl under nanograined (~ 100 nm) form. But this leads to a decrease of its Seebeck coefficient and thus, to poor thermoelectric properties. To understand this opposite effect, we undertook a neutron diffraction experiment (9/9/2020, CRG-2769) on D1B to determine as a function of temperature (25 – 900°C) the crystalline structures adopted by nanograined-Fe2VAl after ball-milling: disordered structures could indeed lead to low Seebeck values. A rapid examination of our data shows that at 25°C, ball-milled Fe2VAl crystallizes in the disordered A2 structure. Upon heating, it orders successively in the B2 and L21 (fully ordered) structures around 300°C - 400°C respectively. Unfortunately, an uncontrollable ramp of the high- temp. furnace prevented us from accurately measuring the temperature of these irreversible transitions. In order to finish this study with publishable data, we hence require an extra beam time (12 – 24h) on D1B equipped with the better controllable 25 - 500°C furnace to measure a new sample prepared under the same conditions.

Easy Access 724, 1/2/2021 : Crystal structures in nanograined-Fe_2VAl polycrystals for thermoelectric applications

E. Alleno, A. Diack Rasselio

Univ. Paris-Est Creteil, ICMPE, UMR CNRS 7182, 2-8, rue H. Dunant, 94320 THIAIS, France

Fe_2VAl could become a good thermoelectric material if its thermal conductivity could be reduced. This can be achieved by synthesizing Fe_2VAl under meso-size grains (~ 1 µm) and well densified polycrystals. But this leads to a decrease of its Seebeck coefficient and thus, to poor thermoelectric properties. To understand this opposite effect, we undertook a neutron diffraction experiment (9/9/2020, CRG-2769) on D1B to determine as a function of temperature (25 – 900°C) the crystalline structures adopted by nanograined-Fe_2VAl after ball-milling: disordered structures could indeed lead to low Seebeck values. A rapid examination of our data shows that at 25°C, ball milled Fe_2VAl crystallizes in the disordered and metastable A2 structure. Upon heating, it orders successively in the B2 and $L2_1$ (fully ordered) structures around 300°C - 400°C respectively. Unfortunately, an uncontrollable ramp of the high- temp. furnace prevented us from accurately measuring the temperature of these irreversible transitions.

The in-situ experiment on a ball milled sample was carried out in the ILL medium-temperature furnace (25 – 550 °C). A 1 K / min ramp was programmed, and this allowed this time to follow precisely the A2 -> B2 and B2 -> $L2_1$ transitions. A plot of the normalised intensity of the 111, 200 and 220 lines is shown in Fig. 1. The 200 line is characteristic of the B2 partial order and the 111 line is characteristic of the $L2_1$ ordered structure. The A2 -> B2 transition occurs at 350 °C whereas the B2 -> $L2_1$ occurs at 550°C.

This implies that sintering the sample at 900 °C fully restores the $L2_1$ structure. As already stated in the CRG N° 2769 report, we finally related the poor Seebeck coefficient of ball milled and sintered samples to a contamination, which modifies the composition.

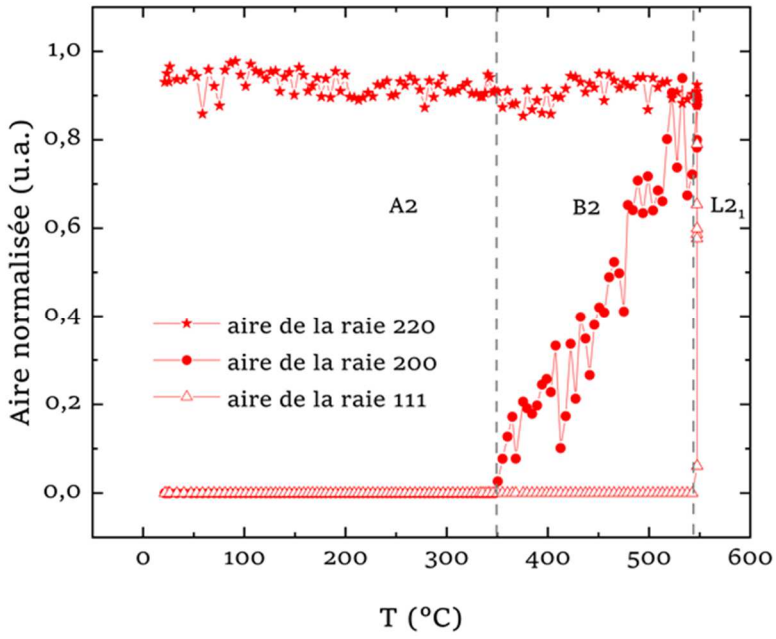

Fig. 1. Normalised integrated intensity of the 111, 200 and 220 lines of ball milled Fe_2VAl versus temperature.