Experimental Report

Proposal: **INTER-277** **Council:** 10/2012

Title: Internal time on D20

This proposal is a new proposal

Researh Area:

Main proposer: **PRYTULIAK Anastasiia**

Experimental Team: PRYTULIAK Anastasiia

Local Contact: HANSEN Thomas

Samples: Mg2Si0.95B0.05

Instrument	Req. Days	All. Days	From	To
D20	1	1	25/06/2013	26/06/2013

Abstract:

Experimental report

Experiment INTER-277
Instrument: D20
Experimental team: A. Prytuliak
Local contact: T. Hansen

Mg_2Si based alloy systems have been actively investigated in order to develop materials which could have good TE properties. Low price and no toxic behavior of these materials are important for the production of TE devices (thermoelectric generators and cooling elements). Moreover, due to low thermal conductivity of these materials it is possible to obtain highly efficient TE materials working in the range of temperatures between 400 – 900K. It is well known that the performance TE materials depends on the figure of merit $ZT = TS^2\sigma/\kappa$, where T, S, σ, and κ are the absolute temperature, Seebeck coefficient, electrical conductivity and total thermal conductivity, respectively.

Over the past five decades, it has been very challenging to increase ZT>1, since the parameters of ZT are so interdependent. For the n-type Mg_2Si based thermoelectrics ZT=1,4 was reached for $Mg_2Si_{0.53}Sn_{0.4}Ge_{0.05}Bi_{0.02}$ composition. Still there is a question to find a p-type counterpart for this material. For this purpose many dopants were tried, boron is one of those, which are theoretically predicted to form p-type material. Unfortunately, it is not obtained experimentally, for this purpose it was important to figure out if boron actually goes into Mg_2Si lattice and if it does, which position it occupies.

$Mg_2Si_{0.53}Sn_{0.4}Ge_{0.05}Bi_{0.02}$ sample was analyzed at room temperature, the wave length was 1.1026 A. It has been find out that sample contains few Mg_2Si based phases and MgO phase, combined refinement of the patterns obtained from neutron diffraction and synchrotron powder diffraction allowed us do get closer to determination of the composition of these Mg2Si base phases. However, as in the sample 4 of the elements are place on the same positions we are facing difficulties to establish exact occupancies.

Besides the sample described above, boron doped sample with nominal composition $Mg_2Si_{0.95}B_{0.05}$ was analyzed up to 600 °C. The absence of pure boron in the sample, as well during the thermal cycling indicates penetration of dopant into Mg_2Si matrix lattice, at the same time an attempts to refine B on Si or interstitial positions give the results of the same reliability.