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EINLADUNG zum IFP-SEMINAR

Microstructure and thermoelectric properties of full-Heusler compounds based on Fe_2VAl co-doped with Ta and Si

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Host: Ernst Bauer

Termin: Mittwoch, 15. April 2020, 16 Uhr

Ort: https://global.gotomeeting.com/join/683902109
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Abstract:

Thermoelectric materials are attractive candidates for recovering waste heat and other sustainable high-end technological applications. Although their thermoelectric figure of merit ZT is relatively low compared to other material classes, Fe_2VAl-based full Heusler compounds have been investigated due to their high power factor that can be attributed to a small pseudogap, where the density of states (DOS) rises sharply in both directions. Nishino et al. showed that Si-doping on the Al-site is an excellent way of optimizing the carrier concentration within the rigid band model [1]. The introduction of Ta atoms on the V-site drastically decreases lattice thermal conductivity as shown by Terazawa et al. [2]. Furthermore, band structure calculations also suggest an opening of the pseudogap and improvement of the electronic structure because of the Ta-doping.
Recently, not so much effort has been put in improving the power factor PF of Fe_2VAl-based compounds as it is already very high. Moreover, a study of the microstructure in the case of Ta/Si-co-doping is still lacking. To find out the solubility limit of Ta and Si and in order to establish a relationship between the microstructure and thermoelectric properties we investigated many different compositions of $Fe_2V_{1-x}Ta_xAl_{1-y}Si_y$ and tuned the annealing conditions.
In this seminar I will discuss the experimental results encompassing XRD and microstructure analysis, as well as the temperature dependence of the Seebeck coefficient S and electrical resistivity ρ in a wide temperature range. SEM images reveal the precipitation of a Ta-/Si-rich impurity phase in some samples leading to a large variety of different microstructures which heavily depend on the annealing durations. The microstructural evolution is strongly tied to the transport properties S and ρ in a nontrivial manner. During the talk, I will manifest an enhancement of the Seebeck coefficient due to the Ta-doping effect as predicted by DFT calculations. Together with an optimization of the microstructure, this yields very high power factors of up to 8 mW/mK2, which is a 50% improvement compared to $Fe_2V_{1-x}Ta_xAl_{1-y}Si_y$ -based compounds from literature [1].

References
1) Y. Nishino IOP Conf. Ser.: Mater. Sci. Eng. 18 142001 (2011)
2) Terazawa et al., Journal of Electronic Materials, Vol. 41, No. 6, 1348, (2012).