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Co-based thermoelectric Heusler alloys: synthesis, transport and magnetic properties

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Waste heat originated by industrial and combustion processes or harvested directly from natural heat sources (i.e. sun, geothermal processes, external heat etc.) can be converted into electricity by means of thermoelectric modules. These devices use the ability of particular materials to convert heat gradients into voltage by means of the so called Seebeck effect. Thermoelectric generators have found applications in aerospace, automotive, sensors, medical, and domestic use; therefore, the study and the optimization of such materials is crucial for achieving higher conversion efficiencies and reducing manufacturing costs.

In this work [1], the thermoelectric and magnetic properties of $Co_2(Zr,Hf)Sn$ alloys were characterized. Arc melted Co_2ZrSn and Co_2HfSn show a uniform matrix of $L2_1$ full-Heusler phase, with small amounts of dispersed secondary phases. Thermoelectric characterization indicated n-type behavior of Seebeck coefficients, with monotonous increasing trends from room temperature to about 450 K followed by plateaus at -33 µV/K and -37 µV/K for Co_2ZrSn and Co_2HfSn, respectively. The electrical conductivity of both Co_2ZrSn and Co_2HfSn show a decreasing trend (i.e., metallic behavior) from room temperature to about 450 K, followed by an increasing trend (i.e., semiconducting behavior). The characterization of magnetic properties was performed by SQUID measurements between 2 and 400 K under a maximum field of 7 T. Sharp hysteresis curves were found for both samples with unsaturated magnetization at high fields. Overall, the alloys were found to show weak ferromagnetic properties suggesting a small separation of majority and minority spin sub-bands in the DOS profile. Magnetic moments per unit formula of 1.81 µB and 2.01 µB were found for Co_2ZrSn and Co_2HfSn, respectively, indicating more remarkable half-metallic ferromagnetic properties for the latter compound. Ab-initio calculations using the VASP code for both alloys were performed. The calculated DOS and band structure also suggested half-metallic ferromagnetic behavior for both the compounds.

[1] *A. Difalco, et al., Metals, 10, 5 (2020), 624.*

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