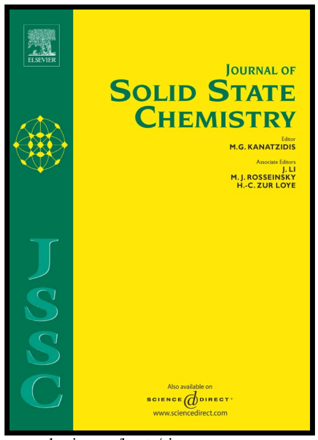

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Microstructure Investigations of Yb- and Bi-doped Mg_2Si Prepared from Metal Hydrides for Thermoelectric Applications

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ABSTRACT

Within the field of thermoelectric materials for energy conversion magnesium silicide, Mg_2Si, is an outstanding candidate due to its low density, abundant constituents and low toxicity. However electronic and thermal tuning of the material is a required necessity to improve its Figure of Merit, *zT*. Doping of Yb via reactive YbH_2 into the structure is performed with the goal of reducing the thermal conductivity. Hydrogen is released as a by-product at high temperature allowing for facile incorporation of Yb into the structure. We report on the properties of Yb- and Bi-doped Mg_2Si prepared with MgH_2 and YbH_2 with the focus on the synthetic conditions, and samples' microstructure, investigated by various electron microscopy techniques. Yb is found in the form of both Yb_3Si_5 inclusions and Yb dopant segregated at the grain boundary substituting for Mg. The addition of 1 at.% Yb concentration reduced the thermal conductivity, providing a value of 30 mW/cm·K at 800 K. In order to adjust carrier concentration, the sample is additionally doped with Bi. The impact of the microstructure on the transport properties of the obtained material is studied. Idealy, the reduction of the thermal conductivity is achieved by doping with Yb and the electronic transport is adjusted by doping with Bi. Large grain microstructure facilitates the electronic transport. However, the synthetic conditions that provide the optimized microstructure for

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