Unique role of refractory Ta alloying in enhancing the figure of merit of NbFeSb thermoelectric materials

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Abstract

NbFeSb based half-Heusler alloys have been recently identified as promising high temperature thermoelectric materials with a figure of merit $zT > 1$, but their thermal conductivity is still relatively high. Alloying Ta at Nb site would be highly desirable because the large mass fluctuation between them could effectively scatter phonons and reduce the lattice thermal conductivity. However, practically it is a great challenge due to the high melting point of refractory Ta. Here we report on the successful synthesis of Ta alloyed (Nb1-xTax)0.8Ti0.2FeSb ($x = 0-0.4$) solid solutions with significantly reduced thermal conductivity by levitation melting. Because of the similar atomic sizes and chemistry of Nb and Ta, the solid solutions exhibit almost unaltered electrical properties. As a result, an overall $zT$ enhancement from 300 K to 1200 K is realized in the single phase Ta alloyed solid solutions, and the compounds with $x = 0.36$ and $0.4$ reach a maximum $zT$ of 1.6 at 1200K. This work also highlights that the isoelectronic substitution by atoms with similar size and chemical nature but large mass difference should reduce the lattice thermal conductivity but maintain good electrical properties in thermoelectric materials, which can be a guide for optimizing the figure of merit by alloying.

Keywords: thermoelectric materials, half, Heusler compound, solid solutions, thermal conductivity

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