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Optimization of the Electronic Band Structure and the Lattice Thermal Conductivity of Solid Solutions According to Simple Calculations: A Canonical Example of the $Mg_2Si_{1-x-y}Ge_xSn_y$ Ternary Solid Solution

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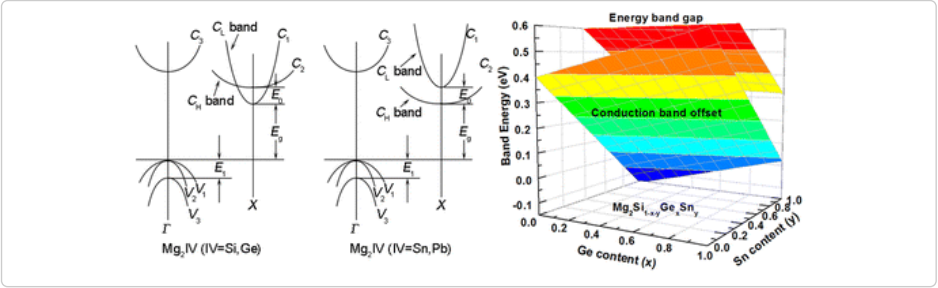
Abstract



The dependence of the electronic band structure of $Mg_2Si_{0.3-x}Ge_xSn_{0.7}$ and $Mg_2Si_{0.3}Ge_ySn_{0.7-y}$ ($0 \le x$, and $y \le 0.05$) ternary solid solutions on composition and temperature is explained by a simple linear model, and the lattice thermal conductivity of solid solutions with different Si/Ge/Sn ratios is predicted by the Adachi model. The experimental results show excellent consistency with the calculations, which suggests that the approach might be suitable for describing the electronic band structure and the lattice thermal conductivity of other solid solutions using these simple calculations. Beyond this, it is observed that the immiscible gap in the $Mg_2Si_{1-x}Sn_x$ binary system is narrowed via the introduction of Mg_2Ge. Moreover, for the Sb-doped solid solutions $Mg_{2.16}(Si_{0.3}Ge_ySn_{0.7-y})_{0.98}Sb_{0.02}$ ($0 \le y \le 0.05$), the energy offset between the light conduction band and the heavy conduction band at higher temperatures (500–800 K) will decrease with an increase in Ge content, thus making a contribution to the conduction band degeneracy and enhancing the power factor in turn. Meanwhile, mass fluctuation and strain field scattering processes are enhanced when Ge is substituted for Sn in $Mg_{2.16}(Si_{0.3}Ge_ySn_{0.7-y})_{0.98}Sb_{0.02}$ ($0 \le y \le 0.05$) because of the large discrepancy between the mass and size of Ge and Sn, and the lattice thermal conductivity is decreased as a consequence. Thus, the thermoelectric performance is improved, with the figure of merit ZT being >1.45 at ~750 K and the average ZT value being between 0.9 and 1.0 in the range of 300–800 K, which is one of the best results for Sb-doped $Mg_2Si_{1-x-y}Ge_xSn_y$ systems with a single phase.

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