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Enhanced Thermoelectric Performance in Cu_2GeSe_3 via (Ag,Ga)-co-doping on cation sites

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Abstract

An enhancement on thermoelectric performance of Cu_2GeSe_3 via simultaneously Ag-alloying on Cu sites and Ga-doping on Ge sites is achieved. The relatively high solubility ($\sim 10\%$) of Ag on Cu sites allows for the strong point defect scattering for phonons, which causes remarkable reduction in lattice thermal conductivity. Ag-rich precipitates emerge when the amount of Ag is higher than the solubility on Cu site, which however do not have significant effect on the lattice thermal conductivity since it is already very close to the lower limit of kinetic theory. Ga-doping, an effective way to tune the hole concentration, leads to optimization of power factor in the whole temperature range. The maximal zT obtained in $\text{Cu}_{1.9}\text{Ag}_{0.1}\text{Ge}_{0.997}\text{Ga}_{0.003}\text{Se}_3$ is $1.03@786\text{ K}$, about 58% higher than that in previous report. In addition, the average zT in the temperature range from 320 K to 786 K is 0.58, implying great potential for fabrication of thermoelectric devices.

Keywords: Thermoelectrics, Cu_2GeSe_3 , Precipitates, Alloying, Doping

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