

Abstract Submitted
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Stronger phonon scattering by larger differences in atomic mass and size in p-type half-Heuslers $\text{Hf}_{1-x}\text{Ti}_x\text{CoSb}_{0.8}\text{Sn}_{0.2}$ XIAO YAN, WEISHU LIU, HUI WANG, SHUO CHEN, Boston College, JUNICHIRO SHIOMI, The University of Tokyo, HENGZHI WANG, DEZHI WANG, Boston College, GANG CHEN, MIT, ZHIFENG REN, Boston College, BOSTON COLLEGE TEAM, MIT COLLABORATION, THE UNIVERSITY OF TOKYO COLLABORATION — High lattice thermal conductivity has been the bottleneck for further improvement of thermoelectric figure-of-merit (ZT) of half-Heuslers (HHs) $\text{Hf}_{1-x}\text{Zr}_x\text{CoSb}_{0.8}\text{Sn}_{0.2}$. Theoretically the high lattice thermal conductivity can be reduced by exploring larger differences in atomic mass and size in the crystal structure. In this paper, we experimentally demonstrated that lower than ever reported thermal conductivity in p-type HHs can indeed be achieved when Ti is used to replace Zr, i.e., $\text{Hf}_{1-x}\text{Ti}_x\text{CoSb}_{0.8}\text{Sn}_{0.2}$, due to larger differences in atomic mass and size between Hf and Ti than Hf and Zr. The highest peak ZT of about 1.1 in the system $\text{Hf}_{1-x}\text{Ti}_x\text{CoSb}_{0.8}\text{Sn}_{0.2}$ ($x=0.1, 0.2, 0.3, \text{ and } 0.5$) was achieved with $x=0.2$ at 800 °C.

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