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Structure and thermoelectric properties of $\text{CoSb}_{3-3X}\text{Ge}_{1.5X}\text{Te}_{1.5X}$ ($X=0 \sim 1$) XIANLI SU, XINFENG TANG, Wuhan University of Technology, CTIRAD UHER, University of Michigan, WUHAN UNIVERSITY OF TECHNOLOGY TEAM, UNIVERSITY OF MICHIGAN TEAM — Changes in the phonon vibration spectra created by substitutions on the rings or by deforming the rings decrease the lattice thermal conductivity. In this research we focused the Ge and Te co-doped and fully compensated $\text{CoSb}_{3-3x}\text{Ge}_{1.5x}\text{Te}_{1.5x}$ skutterudite compounds for the first time. A single-phase skutterudite can be obtained with x smaller than 0.50. In comparison with a ternary skutterudite of the form $\text{CoGe}_{1.5}\text{Te}_{1.5}$, the order-disorder transition can be observed due to the different configuration of four-member pnictogen rings. Rietveld refinement result shows that the bond distance of Sb-Sb decreases with the increase of the Ge and Te content. With x smaller than 0.5, Ge/Te distribute randomly on the four-member near-square Sb rings. For the $\text{CoGe}_{1.5}\text{Te}_{1.5}$ sample, Ge Te distribute in a staggered pattern. Due to the different bonding distance and bonding angle, the near-square ring turns into a parallelogram ring, the essence of the order-disorder transition. The thermal conductivity decreases dramatically with the increasing content of Ge/Te double-doping due to the enhanced alloy scattering.

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