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Thermoelectric Power Factor Enhancement in Tetrahedrites XU LU, Department of Physics & Astronomy, Michigan State University, DONALD MORELLI, Department of Chemical Engineering & Materials Science, Michigan State University, YONGSHENG ZHANG, CHRIS WOLVERTON, Department of Materials Science & Engineering, Northwestern University, MORELLI GROUP IN MSU TEAM, WOLVERTON GROUP IN NORTHWESTERN COLLABORATION
— We report a strategy for power factor enhancement of the thermoelectric properties of $Cu_{12}Sb_4S_{13}$ tetrahedrites. Our previous strategy to improve the figure of merit in tetrahedrites was to reduce the electronic thermal conductivity at the expense of reducing the power factor by replacing monovalent Cu with divalent Zn or Fe. Here, we substitute S with Se, which is isovalent with S and therefore does not induce a doping effect. However, we observe a reduction in electronic resistivity in $Cu_{12}Sb_4S_{13-x}Se_x$ without affecting the thermopower, which leads to at least a 20% enhancement in power factor. Furthermore, the substitution of S with Se causes a reduction in the lattice thermal conductivity via a solid solution effect, keeping the total thermal conductivity unchanged. Density Functional Theory (DFT) calculations indicate a narrowing of the band gap in $Cu_{12}Sb_4Se_{13}$ relative to the sulfide; however, DFT also shows that the pure selenide is not thermodynamically stable. But $Cu_{12}Sb_4S_{13-x}Se_x$ single phase materials may be synthesized up to at least x = 3. We believe this strategy will introduce additional degenerate energy levels near the top of valence band. Further studies should be performed to investigate the optimal Se concentration and its effect on figure of merit.

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