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Synthesis of High Performance Thermoelectric Materials Directly from Natural Mineral XU LU, Department of Physics & Astronomy Michigan State University, DONALD MORELLI, Department of Chemical Engineering & Materials Science Michigan State University, YI XIA, FEI ZHOU, VIDVUDS OZOLINS, Department of Materials Science & Engineering University of California, Los Angeles, HANG CHI, XIAOYUAN ZHOU, CTIRAD UHER, Department of Physics University of Michigan — We report high performance TE materials synthesized directly from natural mineral. Lattice dynamics and electronic band structure calculations suggest that the compound tetrahedrite ($Cu_{12-x}M_xSb_4S_{13}$), where M is transition metal such as Zn or Fe, will have low lattice thermal conductivity and good electronic transport properties. We have experimentally investigated the relationship between ZT and x content of different transition metals in synthetic tetrahedrites. We have found that the maximum of ZT value is not sensitive to the value of x but is related to valence band hole filling fraction; high ZT can be maintained over a large range of x. The compositions studied span the range of those of natural mineral tetrahedrite. To demonstrate that the natural mineral itself can be used as a source material, we synthesized samples by mixing natural mineral with synthetic $Cu_{12}Sb_4S_{13}$ by balling milling and hot pressing. The resulting samples were single phase with hole filling fraction in the optimum range and displayed maximum ZT values of unity at 723K. This new synthesis method can directly use natural mineral to produce TE materials in large quantities with little effort.

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