Synthesis and study of the thermoelectric properties of $CuFeS_2$ doped with P and Sb

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Chalcopyrite is a promising thermoelectric material(TE) due to its low thermal conductivity, non-toxicity, abundance and price. In its native form, low electrical conductivity limits its use as a TE material. We aim to increase its properties with another element substitution. Whereas substitution in cation lattice was widely studied to improve thermoelectric properties, anionic lattice remained unexplored. To study the effects of phosphorus and antimony substitution for sulfur, we prepared polycrystalline samples of P and Sb-doped chalcopyrite with compositions $CuFeS_{2-x}P_x$ and $CuFeS_{2-x}Sb_x$. Synthesis was performed in a resistance furnace from powders (5N purity) with a gradual temperature increase from 300 to 900K. The resulting ingots were grounded in the air. For transport properties measurements, round samples were prepared by hot pressing from synthesized powders. Temperature dependencies of the transport properties were measured and calculated, namely the electrical conductivity, the Hall coefficient, the Seebeck coefficient and the thermal conductivity. In conclusion, we evaluated the effect of substitution in the anionic subgrid on the increase of the ZT parameter. Both phosphorus and antimony led to an increase in the ZT parameter. Newly formed secondary phases are interesting materials for further research.