Microstructure Design Approach to Thermoelectric Materials

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Thermoelectric performance of polycrystalline materials is greatly influenced by their microstructures including grain sizes, grain boundaries, grain orientations in anisotropic compounds, dispersion states of the secondary phase in composites, etc. The material microstructures are sensitive to the preparation processes as well as the starting materials. These make the understanding of the microstructure influence on thermoelectric transport properties very complicated. In the present study, the effect of microstructures in different scales on the thermoelectric properties has been investigated. We synthesized half Heusler-based and skutterudite-based composites using C60, amorphous Si_3N_4, and g-Al_2O_3 particles as the dispersion phases, and Bi_2Te_3-based sintered materials with textured structures. For ZrNiSn-based half-Heuslers or $CoSb_3$-based skutterudites, when dispersion particles are randomly and discretely dispersed in the matrix, ZT values are not enhanced because of power factor reduction even though thermal conductivity is also reduced. When the dispersion particles are dispersed homogeneously on the grain boundaries coating the matrix grains, an enhancement in ZT values is obtained due to a greater reduction of lattice thermal conductivity and an increase of thermopower in spite of somewhat decrease of electrical conductivity. In these samples, the carrier scattering mechanisms are much different than those of the matrix materials. This is considered to be due to the special grain boundary structures. The Bi_2Te_3-based sintered materials with preferred orientations have successfully been fabricated through a spark plasma sintering (SPS) technique by controlling the particle sizes of the starting powders and the sintering process. The obtained textured Bi_2Te_3-based materials show high mechanical strength and significant anisotropy in thermoelectric transport properties. Thermoelectric performance perpendicular to the pressing direction (with c-axis preferred orientation) is comparable to that of single crystal materials in the same crystallographic orientation. It is effective to design and control multi-scale structures for improving thermoelectric performance.