Enhancement of the thermoelectric conversion efficiency of PbTe - based compounds for renewable energy applications

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In the thermoelectric (TE) effect thermal energy is converted into electrical energy and vice-versa. TE devices can, therefore, serve for heat-exchange as well as capturing waste heat and converting it into electricity; the latter has major implications for energy harvesting. The thermal-to-electrical energy conversion efficiency can be improved by reducing the materials’ thermal conductivity, $\kappa$, and/or increasing their electrical conductivity.

The lead-telluride (PbTe) compound is commonly used for TE energy conversion at the mid-temperature range. We investigate the microstructure evolution of PbTe to optimize its TE performance. Experimentally, we focus on the Pb-Te-Ag system, having the potential of forming Ag$_2$Te-precipitates dispersed in a PbTe-based solid solution. The Ag$_2$Te precipitates are expected to serve as phonon scattering centers, thereby reducing lattice thermal conductivity. To achieve significant decrease in $\kappa$, it is required to attain values of precipitate number densities, $N_v$, as high as $10^{20}$ m$^{-3}$.

We prepare ternary (PbTe)$_{1-x}$(Ag$_2$Te)$_x$ alloys with $x = 0.03$ or $0.05$, applying vacuum melting and hot-pressing. We perform homogenization and aging heat treatments at 380, 400, and 450 °C for durations up to 106 h to control nucleation and growth of the Ag$_2$Te-phase. We analyze the precipitates’ number density, volume fraction, and average size employing high-resolution scanning electron microscopy (HRSEM), and find that the precipitates volume fraction keeps growing with aging time, until reaching its equilibrium value. In turn, they undergo growth and nucleation followed by coarsening, which is manifested by non-monotonous variation of number density, exhibiting an optimized value of $N_v = 2 \cdot 10^{20}$ m$^{-3}$ obtained after 6 h aging at 380 °C. We determine the materials’ thermal conductivities using laser-flash analysis (LFA), indicating significant changes associated to microstructure evolution; E.g. the $\kappa$-values measured at 150 °C range between 1.05 and 1.45 Wm$^{-1}$K$^{-1}$ due to aging at 380 °C. We, finally, discuss the interplay between precipitation and the solid-solution degree of super-saturation, and how it affects thermal conductivity. The data acquired in this study help us establish the correlation between a material’s microstructure and composition and its TE performance.

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