PbSe crystal grain boundaries as versatile phonon scatterers

Daniele Selli, Salah E. Boulfelfel, Philipp Schapotschnikow, Davide Donadio, Stefano Leoni

Max Planck Institute for Polymer Research (MPGP) of the Max Planck Society (MPG), Germany

Thermoelectrics are materials of high priority for renewable energy harvesting. In practice however, their applicative use is still limited by their limited efficiency. Engineering materials by alloying and/or nano-structuring so to reduce their thermal conductivity without affecting their electronic features, is a viable route to improve their thermoelectric performances. Hierarchical nanostructuring has been proposed as a an effective way to considerably lower the thermal conductivity of materials. The efficiency of the hierarchical approach lies in the presence of phonon scattering features on a broad range of length-scales, with a consistent reduction of the mean free paths of phonons over the whole spectrum.

Here, by atomistic materials modeling we propose a route to grain engineering in PbSe, using B1-B2 polymorphic transformations as a source of material structuring via domain formation. The transformation of a single crystal into a hierarchical nano-grained structure can be triggered by the rapid application and release of pressure. This procedure gives rise to a material with phononic properties very different from the single crystal precursor, which lead to very low thermal conductivity. Our molecular dynamics simulations elucidate how grains at varying length scales affect thermal transport and phonon scattering.