MEASUREMENTS AND SIMULATIONS OF THE PHONON THERMAL CONDUCTIVITY OF ENTROPY STABILIZED ALLOYS

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The phonon thermal conductivity of solids is intimately related to any changes in atomic scale periodicity. As a classic example, the phonon thermal conductivity of alloys can be greatly reduces as compared to that of the corresponding non-alloy parent materials. However, the improved mechanical properties and environmental stability of alloyed materials makes these multi-atom solids ideal for a wide variety of applications. In this sense, entropy stabilized oxides and high entropy diborides are promising new materials that have potential to withstand extreme environments consisting of high temperatures and pressures. In these novel materials, thermal characterization is essential for understanding and predicting performance at elevated temperatures, as the presence of multi atomic species (5+ different atoms) in these solid solutions could lead to drastically modified phonon scattering rates and thermal conductivities. In this talk, we present recent measurements and molecular dynamics simulations on multiple atom alloys, including entropy stabilized oxides and high entropy diborides. We use time-domain thermoreflectance (TDTR), and optical pump-probe technique, to measure the thermal conductivity of these various systems. We also demonstrate the ability to extend TDTR measurements to temperatures above 1000 deg. C. The TDTR measurements show drastic reductions in the thermal conductivity of these crystalline solid solution materials, approaching values of the amorphous phases. These reductions in thermal conductivity can not be explained by phonon-mass scattering alone. Thus, to investigate the nature of the reduction in thermal conductivity of these multi-atom solid solutions, we turn to classical molecular dynamics simulations. In agreement with the Klemens' perturbation theory, the thermal conductivity reduction due to mass scattering alone is found to reach a critical point, whereby adding more impurity atoms in the solid solution does not reduce the thermal conductivity. A further decrease in thermal conductivity requires a change in local strain-field, which together with mass defect scattering can lead to ultralow thermal conductivities in solid solutions, which surpasses the theoretical minimum limit of the corresponding amorphous phases. These simulations qualitatively agree well with our experimental measurements, and add insight into the nature of phonon scattering in entropy stabilized materials.

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