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

Patrick Hopkins, University of Virginia
phopkins@virginia.edu

Ashutosh Giri, University of Virginia; Jeffrey Braun, University of Virginia; Christina Rost, University of Virginia; Lavina Backman, University of Virginia; Elizabeth Opila, University of Virginia; Mina Lim, North Carolina State University; Zsolt Rack, North Carolina State University; Samuel Daigle, North Carolina State University; Kevin Ferri, North Carolina State University; Trent Borman, North Carolina State University; Jon-Paul Maria, North Carolina State University; Donald Brenner, North Carolina State University; Joshua Gild, University of California, San Diego; Tyler Harrington, University of California San Diego; Jian Luo, University of California, San Diego; Kenneth Vecchio, University of California San Diego; Cormac Toher, Duke University; Pranab Sarker, Duke University; Stefano Curtarolo, Duke University;

Key Words: thermal conductivity, entropy stabilized materials, phonon mass scattering, phonon strain scattering, high temperatures

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 reduced 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.

This work is supported by the U.S. Office of Naval Research MURI program (grant No. N00014-15-1-2863).