THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT
FALL COLLOQUIUM SERIES PRESENTS:

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Origin of unexpectedly low thermal conductivity in Mg_3Sb_2 and Mg_3Bi_2 thermoelectric materials.

In the past five years, Mg_3Sb_2 and Mg_3Bi_2 alloys have emerged as exceptional room-temperature thermoelectric materials, threatening to overthrow the decades-long reign of Bi_2Te_3. The success of these compounds is thanks in large part to their surprisingly low lattice thermal conductivity, which is rarely observed in simple, lightweight compounds. This talk will explore the chemical and thermodynamic origins of the anomalously low thermal conductivity in the Mg_3Pn_2 system (Pn = Sb, Bi). Temperature-dependent measurements of the elastic moduli and first principles phonon calculations were used to investigate the bond strength, rate of softening, and mode Grüneisen parameters. Compared with other isostructural compounds, we find that both Mg_3Sb_2 and Mg_3Bi_2 have anomalously soft shear moduli and large mode Grüneisen parameters. We attribute this behavior primarily to the small size of the Mg cations: Mg is undersized with respect to the 6-fold octahedral coordination environment, leading to weak anharmonic interlayer bonding and high rates of Umklapp phonon-phonon scattering. This is corroborated by the phonon spectra obtained from inelastic neutron scattering of Mg_3Bi_2 and $YbMg_2Bi_2$ single crystals, which show significant softening of the acoustic phonons when Yb is replaced by the smaller Mg cation. In addition, we used *in-situ* high-pressure synchrotron X-ray diffraction to investigate the structure and bonding in Mg3Sb2 and Mg_3Bi_2 at pressures up to 50 GPa. By extracting the pressure-dependent volume change of the polyhedra using Mg_3Sb_2 single crystal diffraction data, we show that the octahedral Mg-Sb bonds are significantly more compressible than the tetrahedral Mg-Sb bonds, lending further support to our argument that the octahedrally-coordinated Mg is responsible for the anomalous thermal properties of the Mg_3Pn_2 system. Further, we report the discovery of a reversible high-pressure phase transition in Mg_3Sb_2 and Mg_3Bi_2 to a monoclinic structure at 7.8 GPa and 4.0 GPa, respectively.

Alexandra Zevalkink joined the Department of Chemical Engineering and Materials Science at Michigan State University as an assistant professor in 2016. She received her B.S. from Michigan Technological University in 2008 and her Ph.D. at the California Institute of Technology in 2014. After completing her Ph.D., she pursued postdoctoral research at NASA's Jet Propulsion Laboratory and at the Max Planck Institute for Chemical Physics of Solids in Dresden, Germany. Her research focus is on the relationship between the atomic structure and bonding in inorganic materials and the resulting elastic, thermal and electronic properties. Her group employs a diverse set of tools including in-situ elasticity measurements, high-pressure and high-temperature X-ray diffraction, and a suite of single crystal growth techniques.

Tuesday, November 17 • 4 pm CT • Zoom

Registration is required. RSVP link is TBD.

Questions? Contact Kristina.lugo@northwestern.edu.

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