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High temperature elastic-moduli as a tool for understanding thermal transport in thermoelectrics

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Abstract: The elastic moduli of solids play a central role in determining functional material properties mediated by phonons. In the study of thermoelectric materials, understanding and controlling the elastic moduli is critical to achieving ultralow lattice thermal conductivity materials. In addition to providing insight into thermal transport, measurements of elastic moduli give us unprecedented sensitivity to local structural changes in materials – whether due to chemical substitutions or temperature-induced phase transitions. Our group uses a resonant ultrasound spectroscopy (RUS) to characterize the elastic moduli of thermoelectrics at temperatures up to 1000°C and single-crystal diffraction in diamond-anvil cells to measure bond-specific compressibility. This talk will cover several recent studies (e.g., 2nd order phase transitions in diamond like semiconductors, anomalous stiffening in GST phase change materials) but the main focus will be on the unprecedented elastic and thermal properties exhibited by Mg3Sb2-based thermoelectrics. Mg3Sb2 shows excellent thermoelectric performance near ambient temperature, enabled by an anomalously low lattice thermal conductivity, comparable to that of much heavier classic semiconductors PbTe and Bi2Te3. Using a combination of resonant ultrasound spectroscopy, inelastic neutron and x-ray scattering, we show that the origin of the low lattice thermal conductivity in Mg3Sb2 is the softening and flattening of its transverse acoustic phonons. Using high-pressure diffraction and first principles calculations, this softening can in turn be traced to a specific Mg-Sb bond. These results provide key insights for manipulating the elastic moduli and phonon scattering of thermoelectric materials, without the traditional reliance on heavy elements.

Biography: 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 and powder metallurgy techniques.