HL 21: Thermal properties

Time: Tuesday 11:00–11:45 Location: POT 361

HL 21.1 Tue 11:00 POT 361

Wigner thermal transport in rare-earth zirconates and their solid solutions — •Anees Pazhedath[1], Lorenzo Bastonero[1], Nicola Marzari[1,2], and Michele Simoncelli[3] — [1]U Bremen Excellence Chair, Bremen Center for Computational Materials Science, and MAPEX Center for Materials and Processes, University of Bremen, D-28359 Bremen, Germany — [2]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [3]Cavendish Laboratory, Theory of Condensed Matter Group, University of Cambridge, England

Anharmonicity and disorder are both limiting factors for heat transport, and understanding how their interplay determines thermal conductivity is crucial to devise design strategies for thermal barrier coatings (TBC). Rare-earth (RE) zirconates are prospective TBC materials, owing to their strong anharmonicity and disorder tunable through alloying. Here, we use the Wigner transport equation in conjunction with state-of-the-art first-principles simulations to elucidate the microscopic physics underlying thermal transport in solid solutions of RE-zirconates, analyzing solutions of $La_2Zr_2O_7$ and $Yb_2Zr_2O_7$ as a paradigmatic test case. This work deepens our understanding on how the interplay between disorder and anharmonicity affects thermal transport in complex crystals with glass-like conductivity, also extending the reach of first-principles simulations to the description of thermal transport in RE-zirconate solid solutions

HL 21.2 Tue 11:15 POT 361

The Influence of Anharmonicity on Negative Thermal Expansion of α-Sn — •Reinhard K. Kremer[1], Paweel T. Jochym[2], Jan Lazewski[2], Andrzej Ptok[2], Przemyslaw Piekarz[2], Andrzej M. Olés[3], and Eva Brücher[1] — [1]MPI for Solid State Research, Stuttgart, Germany — [2]Institute of Nuclear Physics, Polish Academy of Sciences, Krakow, Poland — [3]Institute of Theoretical Physics, Jagiellonian University, Krakow, Poland

The lattice vibrational properties of α-Sn (gray tin) were investigated experimentally by temperature dependent x-ray diffraction and theoretically by density functional theory calculations. Similar to the other elements of group IV, α-Sn exhibits a lattice anomaly at low temperatures and negative thermal expansion, with a minimum at ~ 27 K and a magnitude three times larger than in Si. Influence of anharmonic effects up to 4th order potential terms on the phonon dispersion relations, the lattice parameters, and the thermal expansion coefficient have been tested. The performed analysis gives an excellent agreement with experiment when quartic potential terms are included in the theory. We point out that negative thermal expansion in α-Sn is not driven by anharmonicity of interatomic potential. This resolves the long-standing puzzle in the thermal behavior of α-Sn.

HL 21.3 Tue 11:30 POT 361

Origin of thermal anisotropy in monoclinic $\beta - Ga_2O_3$ — •Markus R. Wagner[1,2], Benjamin M. Janzen[2], Zbigniew Galazka[3], Bartlomiej Graczykowski[4], Kai Xu[5], Ricardo Rurali[5], and Juan Sebastian Reparaz[5] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Technische Universität Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany — [4]Faculty of Physics, Adam Mickiewicz University, Poland — [5]Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Spain

We present a comprehensive all-optical contact-free investigation of the anisotropy of GHz and THz phonon-mediated material properties in $\beta - Ga_2O_3$. The full thermal conductivity tensor is determined by a newly developed all-optical experimental technique that enables sub-degree angular resolution in the measurement of the in-plane anisotropy of the thermal conductivity based on anisotropic frequency-domain thermoreflectance. Using this novel approach we determine the in-plane anisotropy of the thermal conductivity and its anisotropy ratio with high precision. The anisotropy of the sound velocity, elasticity, and Young modulus is measured by polarized, angular-resolved Brillouin light scattering of GHz acoustic phonons. Based on the experimental anisotropy maps of acoustic phonon velocities and thermal conductivity in combination with calculations of the phonon density of states and phonon lifetimes, we discuss the individual contributions of phonon velocities and phonon lifetimes to the anisotropy of the thermal conductivity.