Inelastic Neutron Scattering for Phonon Engineering in Thermoelectric Materials

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Thermoelectric (TE) materials have been researched extensively, particularly in the last decade, with the hope that they will be able to allow for a vast number of impactful and novel technologies to help with the current energy and environmental crises. The challenge of designing a highly performing TE material lies in the requirement to de-couple the electronic and thermal transport; creating a material that has the electronic properties of a highly conducting crystal, while simultaneously having the thermal properties of a poorly conducting glass. The phonon-glass electron-crystal concept has contributed to significant research on the “phonon engineering” of materials. One exceptionally useful tool for aiding this engineering process is inelastic neutron scattering (INS). Information such as phonon linewidth, dispersion, and density of states (DOS), directly obtained by INS, can all be related back to the thermal properties of materials. In this talk, I will give an overview of the usefulness of INS as a tool to study phonons in TE materials by presenting some of our recent INS data on chalcogenide-based TE materials obtained at the Australian Nuclear Science and Technology Organisation (ANSTO). In our work, we explore how INS can be used to understand the thermal conductivity of SnTe, SnSe, and Cu2Se materials by studying the evolution of phonon modes as a function of temperature using ANSTO’s time-of-flight spectrometer, Pelican, and triple-axis spectrometers, Sika and Taipan. Additionally, we compare the phonon DOS of these materials with those of carbon nanomaterials, such as graphene and nanodiamond, to understand phonon scattering rates in C:TE composites due to thermal boundary resistance. We find that carbon nanoparticles act as excellent phonon scatterers because of the large energy mismatch of phonon modes.[1] Finally, we briefly showcase our work which experimentally confirms a recently proposed universal law for the vibrational DOS of liquids, using INS, which provides insight into the complex thermal properties of liquids.[2]

[1] Li, M.; Cortie, D. L.; Liu, J.; Yu, D.; Islam, S. M. K. N.; Zhao, L.; Mitchell, D. R. G.; Mole, R. A.; Cortie, M. B.; Dou, S.; Wang, X., Ultra-high thermoelectric performance in graphene incorporated Cu2Se: Role of mismatching phonon modes. Nano Energy 2018, 53, 993-1002.
[2] Stamper, C.; Cortie, D.; Yue, Z.; Wang, X.; Yu, D., Experimental Confirmation of the Universal Law for the Vibrational Density of States of Liquids. J. Phys. Chem. Lett. 2022, 13 (13), 3105-3111.