Seminar/Talk

Engineering Grain Boundaries in Thermoelectric Materials

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Host: Maria Ibáñez

Engineering Grain Boundaries in Thermoelectric MaterialsGrain boundaries have a remarkable effect on the thermal and electrical transport properties of polycrystalline materials but are often ignored by prevailing physical theories. Grain boundaries and interfaces can adversely alter the properties of Solar Cells, Batteries and Thermoelectrics. To devise strategies for improving the thermoelectric performance of materials, it is essential to understand the coupled charge and thermal transport mechanisms including interfacial electrical and thermal resistance (Kapitza resistance) and even an interfacial Seebeck effect. The inhomogeneous nature of materials, such as that caused by grain boundaries, must be taken into account to rethink engineering strategies based on Mathiessen's rule which interprets scattering homogeneously.Electrical grain boundary resistance can be so high in some thermoelectric materials it is the dominant property that limits zT. While small grains are usually considered beneficial for thermoelectric performance due to reduced thermal conductivity, MgSb based thermoelectric materials, so far at least, contradict that trend. The effect of grain boundary electrical resistance has been more striking and lead to the development of new electronic transport models in granular materials to explain and predict the electrical conductivity. Indeed, atomic segregation has been recently observed at the nanometer scale in grain boundaries in many materials suggesting interfacial or complexion phases should be specifically considered when understanding nearly all thermoelectric materials. These phases can even be engineered not only with thermodynamic quantities such as temperature and composition but also by adding 2D interfacial materials such as graphene. References J. J. Kuo, G. J. Snyder "Grain boundary dominated charge transport in Mg3Sb2-based compounds" Energy & Env. Sci. 11, 429 (2018)R. Hanus, G. J. Snyder "Phonon diffraction and dimensionality crossover in phonon interface scattering" Communications Physics 1, 78 (2018)Y. Lin et al., "Expression of interfacial Seebeck coefficient through grain boundary engineering with multi-layer graphene nanoplatelets". Energy & Environmental Science 13, 4114 (2020).

Thursday, April 14, 2022 10:00am - 11:00am
Big Seminar Room B - Sunstone Building

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