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DEPARTMENT OF
MECHANICAL ENGINEERING
THE UNIVERSITY OF HONG KONG

SEMINAR

Engineering Defects and Grain Boundary for Thermoelectrics

Date: 3 September, 2024 (Tuesday)
Time: 2:45 p.m.
Venue: Room 7-34 & 7-35, Haking Wong Building
HKU

Speaker: Professor G Jeffrey Snyder
Northwestern University
USA

Abstract:

Defects and Grain boundaries have a remarkable effect on the thermal and electrical transport properties of polycrystalline materials but are often ignored by prevailing physical theories. Point defects can be altered with phase boundary mapping and processing engineered with defect thermodynamics. Grain boundaries and interfaces can adversely alter the properties of Power Electronics, Solar Cells, Batteries and Thermoelectrics such as interfacial electrical and thermal resistance (Kapitza resistance) and even an interfacial Seebeck effect. Interfacial thermal resistance limits the performance of power electronics because of overheating. New scanning thermal reflectance techniques can image the thermal resistance of interfaces and boundaries directly. The Thermal conductivity suppression at grain boundaries can even be imaged showing that different grain boundaries can have very different thermal resistances with high energy grain boundaries having more resistance and low energy boundaries having lower thermal resistance.

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, Mg_3Sb_2 based thermoelectric materials, so far at least, contradict that trend. 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.
The concentration of point defects, such as vacancies, interstitial and substitutional atoms can now be predicted with DFT allowing defects to be included in phase diagram analysis for prediction of materials processing for particular properties.

References:

[1] E. Isotta et al., “Microscale Imaging of Thermal Conductivity Suppression at Grain Boundaries”. *Advanced Materials* 2302777 (2023).

[2] J. J. Kuo, G. J. Snyder “Grain boundary dominated charge transport in Mg_3Sb_2-based compounds” *Energy & Env. Sci*. **11,** 429 (2018)

[3] Y. Lin et al., “Expression of interfacial Seebeck coefficient through grain boundary engineering with multi-layer graphene nanoplatelets”. *Energy & Environmental Science* **13**, 4114 (2020).

ALL INTERESTED ARE WELCOME

For further information, please contact Prof. Y. Chen at 3917 7095.