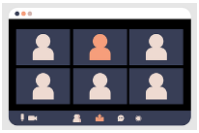
Materials Science Hybrid Colloquium



TECHNISCHE UNIVERSITÄT DARMSTADT

MATERIAL-WISSENSCHAFT

Thursday, May 22, 2025, 15:20, Room 77 & Zoom

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Interface and Grain Boundary Effects on Thermal, Electrical and Magnetic Properties

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. The concentration of point defects can be altered with phase boundary mapping considering the defect thermodynamics. Thus the properties can be engineered with careful processing control.

Grain boundaries and interfaces can adversely alter the thermal and electrical properties of Power Electronics, Solar Cells, Batteries, Thermoelectrics and permanent magnets such as interfacial electrical and thermal resistance (Kapitza resistance). 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.

Interfaces and grain boundaries are 2-dimensional thermodynamic phases (complexions) that have distinct energy, composition and properties that can be rigorously described using the Gibbs excess formalism. The common thermodynamic quantities of temperature and chemical potential connects the complexions to the 3-D phases allowing a phase boundary mapping of grain boundary and interface properties similar to that for point defects.

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 multilayer graphene nanoplatelets”. *Energy & Environmental Science* **13**, 4114 (2020).

4. Leah Borgsmiller, Duncan Zavanelli, and G. Jeffrey Snyder PRX Energy **1**, 022001 (2022)

https://tu-darmstadt.zoom.us/j/64148750805?pwd=eUcyd2M5a1FaWVdiN3ZOR2I2Mm5XUT09

Meeting-ID: 641 4875 0805, Code: 716255