



22nd International Conference on
Diffusion in Solids and Liquids
22 TO 26 JUNE 2026 | RHODES, GREECE

ABSTRACT:

The Origin of Grain Boundary Phase Behavior in Elemental Metals

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Grain boundaries greatly influence many properties of engineering materials. Similarly to bulk materials grain boundaries exhibit phases and first-order phase transitions that result in discontinuous changes in their properties. This talk will focus on recent discoveries of grain boundary phase transitions in elemental metals by modeling and experiments, enabled by the development of new computational tools that perform grand canonical optimization of grain boundary structure. The talk will explain why certain grain boundaries possess unusual quasi-aperiodic ground state structures and undergo first-order phase transitions while others do not. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.