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Modeling Thermodynamics, Kinetics and Defects in Solidification Phenomena Using Phase Field Crystal Methods

Sunday, 28 May 2017 11:45 (30 minutes)

In this talk we first introduce a new extension to the structural phase field crystal (XPFC) approach that employs rotationally invariant multi-point correlation functions which allow for a progression of complex materials phenomena to be simulated, ranging from pressure-induced phase transitions between vapor-liquid-solid phases to polycrystalline solidification and grain growth in both metallic and complex non-metallic solids. New results from two recent studies made using the XPFC modelling will be presented. The first examines defect-assisted nucleation of precipitate solute clusters in ternary alloys (Al-Mg-Si). The second study uses a new XPFC model to examine the role of pressure and on growth rates and defect structures in graphene.

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