



THE HONG KONG UNIVERSITY OF SCIENCE & TECHNOLOGY

Department of Mathematics

PHD STUDENT SEMINAR

A KWC-Based Phase-Field Model for Grain Boundary Grooving

By

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Abstract

Grain boundary (GB) grooving at free surfaces governs thin-film stability and polycrystalline microstructure evolution, yet Mullins' classical theory assumes an isotropic, fixed-energy GB and cannot capture coupling with grain migration or rotation. We propose a new phase-field model that combines the Kobayashi–Warren–Carter (KWC) framework for orientation-resolved polycrystals with a conserved density field evolved by a Cahn–Hilliard equation, so that surface energy, misorientation-dependent GB energy, and the dihedral angle at the groove root all emerge from a single free-energy functional. We validate the model against Mullins' theory, recovering the predicted $t^{\frac{1}{4}}$ groove-deepening kinetics and equilibrium dihedral angle. We then use the model to map the steady-state groove angle as a function of misorientation, and show that the intrinsically nonlinear, Read–Shockley-like GB energy of the KWC formulation is faithfully transmitted to the groove geometry, producing systematic departures from constant-energy predictions. Finally, for curved and embedded grain configurations, we examine the coupled interaction among GB migration, grain rotation, and grooving, demonstrating that the proposed model offers a unified, thermodynamically consistent platform for studying surface–GB coupling beyond the reach of sharp-interface theory.

Date : 14 May 2026, Thursday

Time : 10:00am

Venue : Room 5506 (Lifts 25/26)

All are Welcome!