

The Hong Kong University of Science & Technology

Department of Mathematics

PhD Student Seminar

Continuum Model and Numerical Scheme for Grain Boundaries in Three Dimensions Incorporating Underlying Microstructure

by

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<u>Abstract</u>

We present a continuum model to compute the curved low angle grain boundaries. Our model is an optimization problem with two constraints, the objective function is the grain boundary energy with respect to the dislocation density potential function η , one of the constraints is the Frank's formula with all possible Burgers vectors, another constraint is the symmetry of second derivatives of the dislocation density potential function η . The optimization problem is solved by the augmented Lagrangian multiplier (ALM) algorithm and projection method. Comparisons with atomistic simulation results shows that our energy can deal with interactions and our continuum model can give excellent prediction of the energy and dislocation density of curved low angle boundaries.

Date: Monday, 6 May 2019
Time: 4:00 p.m. - 5:00 p.m.
Venue: LTK, 2/F, Academic Building (near Lifts 31 - 32), HKUST

All are welcome!