Physical Mathematics Seminar

Two Materials Science Applications of the Level-Set Method

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Abstract

I will briefly review the Level-Set Method, originally proposed by Sethian and Osher, and discuss two interesting applications of the method in materials science. The first application is the chemical vapor deposition of diamond. In this problem, we determine the growth rate on different diamond crystal facets using atomistic simulation methods and use these to prescribe the velocity of each facet on each crystal in a polycrystalline sample. We study the evolution of the entire microstructure, its crystallographic texture, surface roughness and grain size. This work was performed with Smereka, Li, and Russo. Next, we propose a new dislocation dynamics simulation method based upon the level-set method. Since dislocations are curves in three dimensions, this is a co-dimension 2 problem. The dislocation dynamics simulations consider anisotropic motion of the dislocations (glide, climb, cross-slip) and full elastic interactions between dislocation segments. We apply this dislocation dynamics method to both dislocations interacting with misfitting particles and the interaction of dislocations to form low-angle grain boundaries. This work was performed with Prof. Yang Xiang.

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