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INTERFACE AND DEFECT DYNAMICS STUDY VIA THE PHASE FIELD CRYSTAL MODEL

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ABSTRACT

The phase field crystal (PFC) model, recently developed by Elder, Grant and co-workers, provides a means for modeling microstructure development from the atomic scale. Unlike other atomic scale techniques, the PFC model operates at diffusive time scales. This opens up for analysis a wide variety of important problems in materials science. However, like any model that resolves at the atomic scale, the model in its original form is limited in size of domain that can be considered by the shear volume of corresponding data and computations.

We present a mathematical reformulation of the PFC model that enables us to solve microscale problems with atomic scale resolution, using a combination of renormalization group analysis and adaptive mesh refinement. The governing equations are recast in terms of the amplitude and phase of the density using two different schemes. In the *Cartesian* form, the equations are recast in terms of the real and imaginary parts of the amplitudes along the crystal basis vectors. We also develop a *polar* form in which the equations are recast instead in terms of the magnitude of the amplitude and the phase. We demonstrate that using a hybrid approach, where we solve the Cartesian form in some parts of the domain and the polar form in the remainder has several computational advantages: (i) the computational domain can be adaptively refined to scales far larger than atomic dimensions; (ii) defects and interfaces can be fully resolved; and (iii) the boundaries separating the two parts of the domain can be resolved seamlessly.

As an example, we placed three seeds of differing orientation in an undercooled melt, comprising a domain approximately $0.75\,\mu\mathrm{m} \times 0.75\,\mu\mathrm{m}$ and allowed them to grow. Fig. 1(Top) shows a sequence of grids from this simulation. The red color indicates the solid, while blue represents the liquid. Fig. 1(Bottom) shows a portion of the grain boundary and through a series of enlargements, one can see that as the crystals intersect, their boundary produces a periodic array of dislocations. In the final enlargement, the density field has been reconstructed, and lines added to indicate the individual dislocations.

We will also present several other example problems, including the development of dislocation arrays in strained layer epitaxial growth, dynamic behavior of dislocation arrays under shear loading, and diffusion in binary alloys.

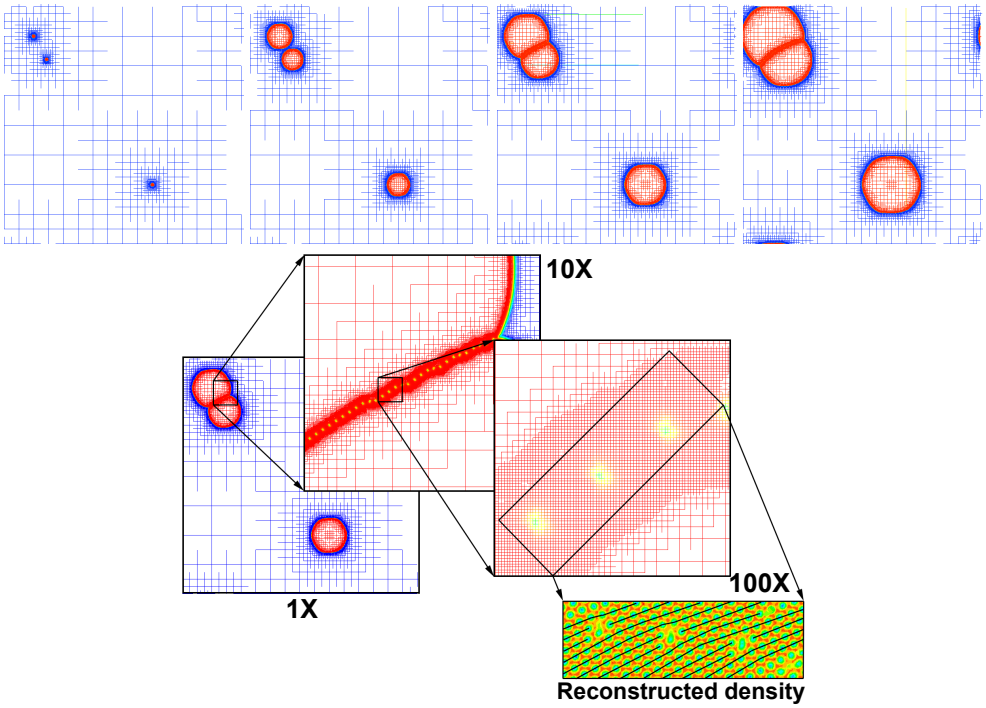

Figure 1: (Top) A sequence of results from a simulation of solidification in an undercooled melt using the hybrid computational scheme. About 100 dislocations are generated in the simulation, mostly found in the grain boundaries. The computational domain is about $0.75\mu\mathrm{m} \times 0.75\mu\mathrm{m}$. (Bottom) Series of enlargements from third panel. The periodic array of dislocations becomes visible at 10X magnification as a series of yellow dots, and a close-up view of three of them is provide in the 100X magnification in reconstructed density form. The dislocations have been highlighted by hand.

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