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A phase field crystal theory of the kinematics and dynamics of dislocation lines

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The Phase Field Crystal (PFC) model is a versatile approach to study the dynamics of defected crystalline materials in terms kinematics and kinetics of dislocations, grain boundaries and fracture dynamics. The PFC model has minimal assumptions based on representing a crystal lattice symmetry by an order parameter that minimizes an appropriate free energy at equilibrium, and that relaxes diffusively in out-of-equilibrium conditions. In this formalism, lattice defects and their properties are determined by the PFC free energy and the dynamics of the order parameter. A challenge with this description is to model dislocation dynamics in the presence of elastic fields and connecting that with continuum elasticity and plasticity descriptions.

In this talk, I will present a general method to identify dislocations in the crystal order parameter and derive expressions for the dislocation density tensor and its dynamics in terms of the evolution of the order parameter. The general expression of the dislocation velocity reduces, under certain approximations, to the overdamped motion driven by the Peach-Koehler force with a mobility determined by equilibrium properties. By extracting the stress tensor in the crystal from the order parameter, we are able to constrain the classical PFC dynamics to mechanical equilibrium. These methods have been used to study the shrinkage of a shear dislocation loop in a bcc lattice which shows that this process depends heavily on state of stress in the crystal.

REFERENCES

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