The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5-9 June 2022, Oslo, Norway

MODELING ELASTIC AND PLASTIC DEFORMATIONS USING THE AMPLITUDE EXPANSION OF THE PHASE-FIELD CRYSTAL MODEL

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Keywords: *Crystals, Phase Field Crystal, Coarse-graining, Elasticity, Plasticity*

The Phase-Field Crystal (PFC) model describes atoms in a lattice through a continuous periodic density field and investigates diffusive time scales. In the amplitude expansion of the PFC model (APFC), a coarse-grained description of this density is obtained by focusing on its complex amplitudes and, in turn, on their dynamics. These amplitudes vary on length scales larger than the atomic spacing but still retain details of the crystal lattice. After outlining the basics of this approach, numerical simulations based on the APFC model and the Finite Element Method are shown to reproduce defects structures in two and three dimensions for different crystal symmetries [1, 2]. The derivation of continuous deformation fields from the complex amplitudes, their connections with the elasticity theory, and the characterization of dislocations are then discussed [3, 4]. Finally, representative applications are shown, such as the prediction of defect motion in binary systems with effects induced by Cottrell Atmospheres [5]. These findings assess the APFC model as a powerful coarse-graining of the PFC model. More importantly, the description of crystal structures through amplitudes emerges as a natural framework connecting atomic-scale lattice deformations and continuum elasticity.

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