



天津大學應用數學中心

Center for Applied Mathematics, Tianjin University

学术报告

An operator-splitting based optimization for phase-field simulation of equilibrium crystals

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摘要: Computing equilibrium shapes of crystals (ESC) is an important problem in materials science. From a mathematical perspective, it can be achieved by minimizing an orientation-dependent (i.e., anisotropic) surface energy functional with a prescribed mass constraint. Especially, when the anisotropic strength is large enough (i.e., strongly anisotropic cases), sharp corners may generate in the ESC even when the surface energy density function is smooth. Direct numerical simulation of this problem via gradient flow can lead to anti-diffusion, which is ill-posed. Traditional technique to resolve this problem is by adding an extra high-order regularization term. However, the resulting dynamics has the effect of penalizing sharp corners, leading to nonphysical solutions. In this talk, we propose

an optimization base approach to minimize the discretized non-regularized phase-field functional under the constraints of mass conservation and bound preservation. In particular, a three-operator-splitting technique is employed and a Davis-Yin splitting (DYS) type algorithm is developed to find the ESC numerically. Numerical experiments show that the proposed method can produce real sharp corners of ESC. Meanwhile, we also prove the global convergence of the numerical solution to the critical point.

欢迎大家参加！