Numerical Methods for Complex Crystalline Materials ASSYR

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Atomistic models are essential in many applications of solid mechanics, such as modeling cracks, structural defects, or nanoelectromechanical systems (NEMS), but full atomistic simulations are prohibitively expensive. Among the efficient methods based on atomistic models, the quasicontinuum (QC) method, introduced by Tadmor, Ortiz, and Phillips, has attracted growing interest in recent years. Originally, the QC method was developed for materials with simple crystalline structure. In the present work we propose an extension of the QC method to complex crystalline materials based on numerical homogenization. We first discuss discrete homogenization, and then formulate and analyze a macro-micro method capable of capturing the effective behavior of the complex material. Numerical examples illustrating the performance of our method will be presented.