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A Numerical Scheme for Generalized Peierls-Nabarro Model of Dislocations Based on the Fast Multipole Method and Iterative Grid Redistribution

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Abstract. Dislocations are line defects in crystalline materials. The Peierls-Nabarro models are hybrid models that incorporate atomic structure of dislocation core into continuum framework. In this paper, we present a numerical method for a generalized Peierls-Nabarro model for curved dislocations, based on the fast multipole method and the iterative grid redistribution. The fast multipole method enables the calculation of the long-range elastic interaction within operations that scale linearly with the total number of grid points. The iterative grid redistribution places more mesh nodes in the regions around the dislocations than in the rest of the domain, thus increases the accuracy and efficiency. This numerical scheme improves the available numerical methods in the literature in which the long-range elastic interactions are calculated directly from summations in the physical domains; and is more flexible to handle problems with general boundary conditions compared with the previous FFT based method which applies only under periodic boundary conditions. Numerical examples using this method on the core structures of dislocations in Al and Cu and in epitaxial thin films are presented.

AMS subject classifications: 65R20, 65N50, 74A50, 74G65

Key words: Dislocation, elasticity, Peierls-Nabarro model, iterative grid redistribution, fast multipole method.

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1 Introduction

Dislocations are line defects and the primary carriers of plastic deformation in crystalline materials. In the dislocation theory, the elastic field of a dislocation is very well described by the continuum linear elasticity theory outside a small region surrounding the dislocation [1]. Inside the small region around the dislocation, which is known as the core region of the dislocation, the atomic structure is heavily distorted, and the linear elasticity theory gives unphysical singularities in the elastic field. The core region determines the energy and the mobility of the dislocation, thus its modeling plays important roles in the dislocation and plasticity theories. The Peierls-Nabarro model [1–3] provides a way to incorporates atomic features inside the core region into the continuum linear elasticity theory. More accurate first principles results can also be included in the framework of the Peierls-Nabarro model [5,10–12,15,17] through the generalized stacking fault energy [4].

In the Peierls-Nabarro model [1–3], the solid is divided by the slip plane of the dislocation into two half-space linear elastic continua, with a disregistry (or misfit) relative to each other and connected by a nonlinear potential force. The total energy consists of the elastic energy in the two half-space continua and the misfit energy due to the nonlinear atomic interaction across the slip plane. The dislocation core profile is determined by energy minimization. The solution of the Peierls-Nabarro model gives a description for the dislocation core profile as well as the energy barrier (Peierls energy) and the critical stress (Peierls stress) for the motion of dislocations. Previously, efforts were made mainly on straight dislocations [2–15,17,19,20].

Several generalized Peierls-Nabarro models for curved dislocations have been proposed [16, 18, 21–23]. Some recent applications of the Peierls-Nabarro models can be found, e.g., in [24–29]. The major numerical challenge of such models lies in the calculation of the long-range elastic interaction. In the finite element based model proposed in [16], this long-range interaction is calculated by direct summation over all the grid points, which requires $\mathcal{O}(N^2)$ operations, where N is the total number of grid points [30]. The lattice model presented in [18] also requires $\mathcal{O}(N^2)$ direct summation for the long-range interaction of dislocation over the slip plane with N lattice sites. The models proposed in [21–23] employ the fast Fourier transform method (FFT) for the generalized Peierls-Nabarro on a uniform mesh with periodic boundary conditions, thus only $\mathcal{O}(N\log N)$ operations are needed for the calculation of this long-range interaction. Although the FFT based generalized Peierls-Nabarro models are quite efficient, they are limited to periodic boundary conditions which mimic the behavior of dislocations in bulk of the materials. However, the periodic boundary conditions cannot be used when materials boundaries are present, for example, when dislocations are in thin films where traction-free boundary conditions are required on the free surfaces [6,7].

In this paper, we present an alternative numerical method for the generalized Peierls-Nabarro model in Ref. [21] based on the fast multipole method (FMM) [33,34] and the iterative grid redistribution [35]. This presented numerical method is an improvement of the available numerical methods in the literature in which the long-range elastic interac-