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Fast Multipole Accelerated Boundary Integral Equation Method for Evaluating the Stress Field Associated with Dislocations in a Finite Medium

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Abstract. In this paper, we develop an efficient numerical method based on the boundary integral equation formulation and new version of fast multipole method to solve the boundary value problem for the stress field associated with dislocations in a finite medium. Numerical examples are presented to examine the influence from material boundaries on dislocations.

AMS subject classifications: 74S15, 65R20, 74A10, 74B05

Key words: Fast multipole method, boundary integral equation method, dislocation dynamics, stress.

1 Introduction

The collective motion and interaction of large numbers of dislocations (line defects) play central roles in the plastic deformation of crystals [1]. The direct numerical simulation of interaction and motion of dislocations, known as dislocation dynamics, is becoming a more and more important tool for the investigation of the plastic properties of crystalline materials [2–26]. However, in order for dislocation dynamics to be a practical engineering tool, large ensembles of dislocations are required in the simulations, which are still beyond the capability of currently available dislocation dynamics methods.

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One of the major limitations of the current dislocation dynamics methods lies in the computational cost for the complex, long-range elastic interactions of dislocations that depend on the relative positions of dislocations, their orientations as well as their Burgers vectors. When a direct method is applied to find the summation of interactions between dislocation segments in numerical discretization of dislocations, the calculation is inherently time consuming and requires $\mathcal{O}(N^2)$ operations, where N is the total number of dislocation segments. Employing cut-off distance is known to produce spurious results [2,4]. Several fast numerical algorithms for the long-range interaction of dislocations in dislocation dynamics simulations have been introduced to reduce the computational cost to achieve the asymptotically optimal $\mathcal{O}(N)$ efficiency [4,6,11,17,21,23,26]. Previously in [26], we have applied the new version of fast multipole method (FMM) [27] to compute the stress field of dislocation ensembles in an infinite medium. Numerical experiments showed that for a dislocation ensemble discretized into N dislocation segments, the new version FMM based method is asymptotically $\mathcal{O}(N)$ with an optimized prefactor and is very efficient for prescribed accuracy requirements.

For materials with boundaries such as thin film materials, there are interactions between dislocations and material boundaries, resulting in image forces on dislocations. Analytical formulas for the image forces are only available for some special cases, e.g., some straight dislocations in half space with a planar free surface [1]. Generally, a complementary stress field should be obtained to satisfy the given boundary conditions, e.g., the traction free boundary conditions [28]. The superposition of the (a) stress field associated with the dislocations in an infinite elastic medium and (b) stress field obtained from solving the boundary value problem without dislocations gives the correct stress field in the finite medium containing dislocations. In most existing simulations, the complementary problem is solved by the finite element method (FEM) [10,12,14,22]. For the special cases of a half space with a planar free surface, Green's function method or FFT are used to solve the boundary value problem [5,7,18,19]; and there are also techniques to include the image forces based on prismatic loops [13,16].

The boundary integral equation method (BIEM) [29] (also called the boundary element method) was developed shortly after the introduction of the finite element methods (FEM) in the 1950s. Compared with the volume discretization in the FEM, BIEM only requires the discretization of the surface and the number of unknowns and required memory are therefore much less than those in the FEM. When applied to dislocation dynamics, once the information on the surface is solved, BIEM is able to evaluate the driving force on dislocations accurately at any point inside the medium, whereas in the FEM, interpolation is needed from the values on the prescribed numerical grid points in the volume discretization. However, as the matrix of the resulting linear system in BIEM is dense, for a problem with N unknowns, when Gauss elimination is applied, $\mathcal{O}(N^3)$ operations and $\mathcal{O}(N^2)$ memory are required. The huge computational cost and storage requirement quickly exhaust the computer resources when $N>10^4$ and the BIEM was less competitive compared with the multigrid and/or domain decomposition accelerated FEM. In the last twenty years or so, to break this bottleneck, by observing the special structure of the ma-