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Boundary Condition for Dislocation Dynamic Simulation in BCC Crystal

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Abstract. The movement of dislocations and the corresponding crystal plastic deformation are highly influenced by the interaction between dislocations and nearby free surfaces. The boundary condition for inclination angle θ_{inc} which indicates the relation between a dislocation line and the surface is one of the key ingredients in the dislocation dynamic simulations. In this paper, we first present a systematical study on θ_{inc} by molecular static simulations in BCC-irons samples. We also study the inclination angle by using molecular dynamic simulations. A continuum description of inclination angle in both static and dynamic cases is derived based on Onsager's variational principle. We show that the results obtained from continuum description are in good agreement with the molecular simulations. These results can serve as boundary conditions for dislocation dynamics simulations.

AMS subject classifications: 65G05, 70G75

Key words: Dislocation, dislocation dynamics, boundary conditions, analytical model, Onsager's variational principle.

1 Introduction

It is widely agreed that dislocations are the main carrier of plastic deformation in crystalline materials. The movement of dislocations is the key mechanism of strain energy relaxation which is highly influenced by the interaction with other defects, external loads and crystal structures [1–6]. Therefore it is important to note that the development of

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an accurate plasticity theory should based on the detailed dislocation mechanics that the movement of each dislocation could be traced, rather than on empirical assumptions [1, 7]. However, as it is well-known that current models of dislocation need to consider phenomenon in multiple scales, i.e., the elastic interactions of dislocations are usually long range, but meanwhile, many other dislocation interactions such as self-force, annihilation, reaction, and multiplication are short range since these effects are highly depending on the local properties dislocation structure. Current simulation techniques which could track the movement of each dislocation in material are usually too complicated due to the multi-scale nature in the description of dislocations, therefore, more comprehensive models are needed to provide more accurate and efficient descriptions of the collective movement of dislocations.

During the last several decades, dislocation dynamics (DD) simulation, which can simulate the movements and interactions of large ensemble of dislocations by direct tracking the dynamics of individual discrete dislocation, were developed to deal with the complicated interactions as well as the pattern evolution of dislocations occurring in the plastic deformation [8–12]. DD simulation now is the most promising tool for the study of dislocations in crystalline materials in mesoscopic scale [13–41].

DD simulation have been successfully adopted to study various phenomenon in crystal plasticity at small scale, for instance, strain hardening effects in cubic or hexagonal crystals [22, 23, 30, 38], microstructure in cyclic deformation [36], plasticity in polycrystalline materials [37]. However, in current conventional DD simulations, the periodic boundary condition is most useful boundary condition for simulation cell in order to calculate the stress due to dislocations based on stress expression in infinite medium [15], it is still a non-trivial task for DD simulations to account the effects of various boundary conditions [42]. How to account the effects induced by various boundaries such as free surfaces in simulations accurately and efficiently is still a crucial problem in the developing of sophisticated DD simulations.

The effect of boundaries such as free surfaces is introduced by the image stress. The image stress is an additional stress in order to guarantee the traction-free boundary condition, which can be calculated based on instantaneous dislocation configuration [1]. In DD simulations, the movements of dislocation segments are determined by the total stress including the image stress, the self stress, the stress due to dislocations and other defects, and the external applied stress. One general approach [13] adopted in calculating the total stress is that the stress is decomposed into two parts, one is the stress due to dislocation ensemble in infinite medium which could be obtained based on classical dislocation theory, and the other one comes from the effects of boundary conditions, i.e., the image stress, which could be solved by using some continuum theories such as finite element method (FEM) or boundary element method (BEM) [13, 17–19, 25, 29, 34]. Many models derived from this approach have been widely used in the study of crystal plasticity [31, 39–41]. These models work well when dislocation segments are relatively away from the free surfaces. However, the image stress due to the boundary are singular when these dislocations approach to and/or intersect with the free surfaces [14,21,25,31,40,42],