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A Generalized Peierls-Nabarro Model for Curved Dislocations Using Discrete Fourier Transform

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Abstract. In this paper, we present a generalized Peierls-Nabarro model for curved dislocations using the discrete Fourier transform. In our model, the total energy is expressed in terms of the disregistry at the discrete lattice sites on the slip plane, and the elastic energy is obtained efficiently within the continuum framework using the discrete Fourier transform. Our model directly incorporates into the total energy both the Peierls energy for the motion of straight dislocations and the second Peierls energy for kink migration. The discreteness in both the elastic energy and the misfit energy, the full long-range elastic interaction for curved dislocations, and the changes of core and kink profiles with respect to the location of the dislocation or the kink are all included in our model. The model is presented for crystals with simple cubic lattice. Simulation results on the dislocation structure, Peierls energies and Peierls stresses of both straight and kinked dislocations are reported. These results qualitatively agree with those from experiments and atomistic simulations.

AMS subject classifications: 35Q72, 65D05, 74C99, 74G65, 74S25

Key words: Dislocation, Peierls-Nabarro model, Peierls stress, Peierls energy, dislocation kink.

1 Introduction

Dislocations are one-dimensional topological defects in crystalline solids, whose motion is directly responsible for the plastic deformation of these materials [1]. When a straight

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dislocation moves in its slip plane over the crystal lattice, its energy changes periodically, and an energy barrier has to be overcome when it moves from one energy valley to another. This energy barrier is referred to as the Peierls energy, and the minimum stress to drive the dislocation over this energy barrier is the Peierls stress [1–4]. In reality, due to thermal fluctuations and other effects, a dislocation line may lie in different Peierls valleys connected by kinks, and the motion of the dislocation is also controlled by the kink nucleation and migration. The energy barrier and the minimum stress to move an individual kink are the second Peierls energy and the second Peierls stress, respectively [1, 5–12]. These Peierls energies and Peierls stresses play important roles in characterizing the mobility of dislocation lines [1–16, 18–30].

The Peierls energy and Peierls stress can be estimated using the Peierls-Nabarro model [1–4], which is a hybrid model incorporating atomic features into continuum framework. In the Peierls-Nabarro model, the solid is divided by the slip plane of the dislocation into two half-space linear elastic continua, which have a disregistry (or misfit) relative to each other and are 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 minimum energy state gives the dislocation core profile on the slip plane. The change of the energy as the dislocation moves over the crystal lattice is obtained by shifting rigidly the continuous dislocation profile and summing the misfit energy over the discrete lattice sites near the slip plane. The Peierls energy is the difference between the maximum and minimum of this discrete summation of misfit energy, and the Peierls stress is associated with the maximum derivative of this discrete summation of misfit energy.

The estimates of the Peierls energy and Peierls stress within the Peierls-Nabarro model give qualitative descriptions for the energy barrier and minimum stress required when the dislocations move over the crystal lattice, and agree reasonably with the experimental results [1–4, 14–16]. The Peierls-Nabarro model has been improved greatly with the generalized stacking fault energy [17] obtained using *ab initio* calculations [18–23]. However, in most of these models, the estimates of the Peierls energy and Peierls stress are still obtained in the same way as those in the classical Peierls-Nabarro model, which has been criticized for the following limitations [20, 25]. The first limitation is the inconsistency in the incorporation of the lattice discreteness: on one hand, the continuous dislocation core profile is obtained from energy minimization, on the other hand, discrete sum is used to calculate the Peierls energy; i.e., the Peierls energy is not directly included in the energy minimization. Another limitation is that only the discreteness of the misfit energy is considered, while the discreteness of the elastic energy is neglected. Finally, this method is based on the assumption that the dislocation core profile does not change as it moves. It has been shown that these limitations may result in large errors especially in dealing with dislocations with narrow cores (e.g. in silicon) [20, 25].

Several efforts have been made to address these problems. Bulatov and Kaxiras proposed a semidiscrete variational Peierls framework [20], in which the total energy is minimized with respect to the disregistry at discrete lattice sites and the elastic energy is still