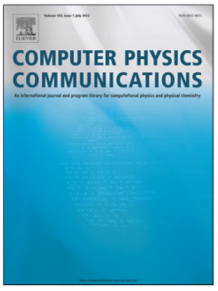
Accepted Manuscript



Acceleration of the Particle Swarm Optimization for Peierls–Nabarro modeling of dislocations in conventional and high-entropy alloys

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PII: S0010-4655(17)30034-6
DOI: http://dx.doi.org/10.1016/j.cpc.2017.01.022
Reference: COMPHY 6140

To appear in: *Computer Physics Communications*

Received date : 24 December 2016
Revised date : 24 January 2017
Accepted date : 25 January 2017

Please cite this article as: Z. Pei, M. Eisenbach, Acceleration of the Particle Swarm Optimization for Peierls–Nabarro modeling of dislocations in conventional and high-entropy alloys, *Computer Physics Communications* (2017), http://dx.doi.org/10.1016/j.cpc.2017.01.022.

Acceleration of the Particle Swarm Optimization for Peierls-Nabarro modeling of dislocations in conventional and high-entropy alloys ☆

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Abstract

Dislocations are among the most important defects in determining the mechanical properties of both conventional alloys and high-entropy alloys. The Peierls-Nabarro model supplies an efficient pathway to their geometries and mobility. The difficulty in solving the integro-differential Peierls-Nabarro equation is how to effectively avoid the local minima in the energy landscape of a dislocation core. Among the other methods to optimize the dislocation core structures, we choose the algorithm of Particle Swarm Optimization, an algorithm that simulates the social behaviors of organisms. By employing more particles (bigger swarm) and more iterative steps (allowing them to explore for longer time), the local minima can be effectively avoided. But this would require more computational cost. The advantage of this algorithm is that it is readily parallelized in modern high computing architecture. We demonstrate the performance of our parallelized algorithm scales linearly with the number of employed cores.

Keywords: Peierls-Nabarro model, dislocations, Particle Swarm Optimization, acceleration

1. Introduction

Dislocations are one of the most important classes of defects that dominate the mechanical properties of crystalline solids [1, 2]. Since it was proposed to explain the huge discrepancy between theoretically predicted and experimentally measured resolved shear stresses of materials, the primary pathway to study dislocations had been experimental methods. With the advance of computing and computational sciences, theoretical simulations of dislocations have emerged as a complementary approach to systematic crystal mechanical experiments to gain insight into the deformation mechanisms [3, 4, 5, 6, 7]. Additionally, when the knowledge of atomic-scale dislocation core structures are critical, theoretical simulations are particularly useful [5, 8, 9, 10]. As examples, Yasi et al. [5] simulated the core structures of basal and prismatic dislocations in Mg using density functional theory (DFT). Later the same authors developed different models to calculate the critical resolved shear stresses (CRSS) of basal dislocations in Mg alloys [11] and the cross-slip stresses of prismatic screw dislocations in Mg [12]. As another example, Shin and Carter applied orbital-free density functional theory (OFDFT) method to model dislocation core structures [6] and subsequently also calculated Peierls stresses in pure Mg [10].

The common feature of the aforementioned atomic-scale simulations is that dislocation cores are described explicitly in an atom-by-atom manner. We refer the methods employed as direct methods. Within this group of methods, the dislocation core structures are relaxed by molecular statics/dynamics simulations using either empirical embedded-atom-method (EAM) potentials [3] or DFT [13, 14]. While the DFT based methods are accurate they are computationally very expensive for simulating dislocations that require usually several hundreds of atoms or even many more due to their long-range fields. Atomistic simulations are efficient but very often there are no reliable EAM potentials for the materials systems of interest.

In contrast to the direct methods, indirect methods do not describe dislocation core structures explicitly by using misfit functions (denoted by u in this work). A misfit function quantifies the distribution of the Burgers vector of a dislocation in space coordinate, i.e., the geometry of a dislocation core. It can be obtained from the Peierls-Nabarro model that was proposed by Peierls and Nabarro [15, 16, 17] about seventy years ago. The original model is applicable for one-dimensional dislocation cores. Later, Leibfried and Dietze generalized the one-dimensional model to two-dimensional case that can address dissociated planar dislocation cores [18]. The primary input is taken from the generalized stacking fault energies (GSFEs,

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