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 al-

loys [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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Figure 1: The two components (u_x, u_z) of the misfit function of basal $\langle a \rangle$ dislocation in Mg and their derivatives (ρ_x, ρ_z). The dislocation is placed in a coordinate as shown in the inset, i.e., the dislocation line runs along z axis, and the slip plane is xz plane. The z axis is perpendicular to the paper.

so-called gamma surface) proposed by Vitek [19]. The gamma surface can be accurately calculated by DFT methods with computationally available and acceptable cost. Therefore, Peierls-Nabarro modeling represents an alternative to the above discussed direct fully atomistic simulation methods for dislocations with planar core structures. In the last years these models have been substantially improved and optimized. For example, Wang added gradients of the misfit density to the total energy functional of dislocations in order to address dislocations possessing narrow cores [20]. The misfit density refers to the first derivative of misfit function with respect to a space variable, which will be discussed in more detail below. Bulatov *et al.* [21] discretized the misfit density and employed an array of discrete data points to describe it (for an application example in Al, see [22]), since the discretized functions can provide more flexibility than the analytic (arctan-type) functions.

The choice of a suitable variant of Peierls-Nabarro model (i.e., a suitable form for the trial solution) depends on the specific problem to be addressed. For example, the dislocation core structures in Mg are usually very complicated, but the basal dislocation has a dissociated planar core, which can be adequately described by four actan functions using the standard two-dimensional Peierls-Nabarro model [7]. For dislocations with significantly narrower cores, more arctan functions are usually required.

2. Peierls-Nabarro Model

In the framework of classical Peierls-Nabarro model, the equilibrium configuration of a dislocation is determined by the balance of restoring force and elastic resistance of the crystal lattice. Here we assume an edge dislocation aligned with the Cartesian coordinate system. The dislocation line goes along the z axis (for screw dislocation the dislocation line runs along the x axis) and its Burgers vector $\vec{b}$ is parallel to x (see Figure

1). Such a dislocation is described mathematically by

$$2K \int_{-\infty}^{+\infty} \frac{\vec{\rho}(x')}{x - x'} dx' = -\frac{d\gamma(\vec{u})}{d\vec{u}} \quad (1)$$

where the left side is the elastic resistance and the right side represents the restoring forces. Specifically $\vec{u}$ is the misfit function and $\vec{\rho}(x)$ is the misfit density, $\vec{\rho}(x) = d\vec{u}(x)/dx$. The generalized stacking fault energy, $\gamma(\vec{u})$, or gamma surface (see Section 2.1), is the key input quantity of the model. In the two dimensional case, the misfit function $\vec{u}$ is a two-dimensional vector consisting of components along x and z , i.e., u_x and u_z respectively. Further, the energy factor K is a proportionality that is in elastically isotropic materials related to the shear modulus μ and the Poisson ratio ν . $K = K_e = \mu/4\pi(1 - \nu)$ for edge dislocations and $K = K_s = \mu/4\pi$ for screw dislocations. The subscripts "e" and "s" in K_e and K_s indicate whether the constant is for an edge or a screw dislocation. In elastically anisotropic media, K depends on the slip system and dislocation character and is calculated from elastic constants. For a basal $\langle a \rangle$ edge/screw dislocation in hexagonal close-packed materials, $K_e = 1/4\pi(\bar{C}_{11} + C_{13})((C_{44}(\bar{C}_{11} - C_{13}))/C_{33}(\bar{C}_{11} + C_{13} + 2C_{44}))^{1/2}$, $\bar{C}_{11} = (C_{11}C_{33})^{1/2}$; $K_s = 1/4\pi(C_{44}C_{66})^{1/2}$, $C_{66} = (C_{11} - C_{12})/2$ [1].

An analytical solution of $\vec{u}$ determined by Eq. 1 exists only for rather simple gamma surfaces. When a gamma surface is described by one cosine function, the exact solution is one arctan function. A dislocation described by one arctan-type function is called Peierls dislocation. For more complex (and more realistic) gamma surfaces, solutions can be obtained only numerically. Often, the solution is obtained by expanding $\vec{u}$ into a series of arctan functions [17]. The arctan function is a suitable basis since it captures the main characters of a dislocation. As an example for an edge dislocation of Burgers vector $\vec{b}$, the misfit function $\vec{u} = (u_e, u_s)$,

$$u_e = \frac{b}{\pi} \sum_i A_i \arctan\left(\frac{x - d_{e,i}}{w_{e,i}}\right) + \frac{b}{2}, \quad \sum_i A_i = 1; \quad (2a)$$

$$u_s = \frac{b}{\pi} \sum_i B_i \arctan\left(\frac{x - d_{s,i}}{w_{s,i}}\right), \quad \sum_i B_i = 0. \quad (2b)$$

where A_i, B_i determine the weights of Peierls dislocations, $d_{e,i}, d_{s,i}$ and $w_{e,i}, w_{s,i}$ characterize the position and half-width of the Peierls dislocations. The subscript differentiates the edge component from the screw component.

By proposing the solution in the form of trial functions as suggested in Eq. 2 and applying the variational principle we transform the integral-differential Eq. 1 into an optimization problem. The left part of Eq. 1 is transformed into the elastic

Table 1: (**Algorithm 1**) The self-consistent procedure to solve Peierls-Nabarro equation.

1:	select a suitable dislocation core radius R
2:	select a suitable trial function for misfit function $u(w_i, A_i, B_i, r_{ij})$
3:	calculate $E_{el}(R; w_i, A_i, B_i, r_{ij})$ using Eq.3
4:	for k in $(-R, R)$ do
5:	calculate $E_A(k; u)$ using Eq.4
6:	$E_c \leftarrow E_c + E(k); E(k) \leftarrow E_{el}(R) + E_A(k)$
7:	end for
8:	adjust u and repeat 3-7 until E_c finds the global minimum
9:	adjust R and repeat 2-8 until u does not change

energy E_{el} [17],

$$\begin{aligned}
 E_{el} = & H_{11} \left(\sum_{i,j} A_i A_j \ln \left(\frac{R}{w_{e,i} + w_{e,j}} \right) - \sum_{i < j} A_i A_j \ln \left(1 + \frac{r_{e,ij}^2}{(w_{e,i} + w_{e,j})^2} \right) \right) \\
 & + H_{33} \left(\sum_{i,j} B_i B_j \ln \left(\frac{R}{w_{s,i} + w_{s,j}} \right) - \sum_{i < j} B_i B_j \ln \left(1 + \frac{r_{s,ij}^2}{(w_{s,i} + w_{s,j})^2} \right) \right) \\
 & + 2H_{13} \left(\sum_{i,j} A_i B_j \ln \left(\frac{R}{w_{e,i} + w_{s,j}} \right) - \frac{1}{2} \sum_{i,j} A_i B_j \ln \left(1 + \frac{r_{ij}^2}{(w_{e,i} + w_{s,j})^2} \right) \right)
 \end{aligned} \quad (3)$$

In this expression H is the Stroh tensor. The terms in the first bracket represent the elastic energy of the edge component, the second stands for the elastic energy of the screw component. $\{H_{11}, H_{33}\} = \{K_e, K_s\}$. The last two terms in Eq. 3 vanish when the dislocation core structure is symmetric, which is actually the cases for basal dislocations in hcp or $\{111\} < 1\bar{1}0 >$ dislocations in face-centered cubic (fcc) crystalline solids. R is the outer cutoff radius, r_{ij} is the distance between edge component of Peierls dislocation j and screw component of Peierls dislocation i , and $r_{e,ij}$ or $r_{s,ij}$ is the distance between the edge or screw components of the Peierls dislocations i and j .

The right part is transformed into the misfit energy E_A , i.e., the integral of the gamma surface within the core region of a dislocation

$$E_A = \int_{-R}^R \gamma(u_x(x), u_z(x)) dx. \quad (4)$$

The Peierls stress τ_p is taken as the maximum of the gradient of the misfit energy E_A , i.e., $\tau_p = \max\{\frac{dE_A}{du}\}$. Since the stress field far away from the dislocation core does not affect the core structure, a large but finite R is sufficient for the evaluation. A larger R does not change the numerical solutions. The total energy of a dislocation is the sum of the misfit energy and the elastic energy,

$$E_{tot} = E_{el} + E_A. \quad (5)$$

Minimizing the total energy E_{tot} to create a dislocation is equivalent to solve Eq. 1. Minimization of E_{tot} (Eq. 5) yields the geometry (characterized by the parameters w and d) of the studied dislocations. We summarize the self-consistent procedure to solve the Peierls-Nabarro equation in Table 1. For conducting the minimization we use the algorithm of Particle Swarm Optimization, since this algorithm can effectively avoid local

Figure 2: Convergence of the Peierls stress of the $\langle a \rangle$ -type edge dislocation in pure Mg and Mg-Y as a function of the plane wave cutoff [7].

minima in the solution space and identify the optimal solution [23, 24, 25]. The details and performance of the algorithm are described in Sections 3 and 4.

In our previous study [7], we focused on $\langle a \rangle$ -type edge dislocations in Mg alloys that are known to dissociate into two partials separated by wide stacking faults [5, 7]. This type of dislocations can be well described by only four arctan functions, i.e., two for the edge component and two for the screw component. The misfit functions Eq. 2 are then written as follows

$$u_x(x) = \frac{b}{2\pi} \arctan \frac{x - d_e/2}{w_e} + \frac{b}{2\pi} \arctan \frac{x + d_e/2}{w_e} + \frac{b}{2}; \quad (6a)$$

$$u_z(x) = \frac{\sqrt{3}b}{6\pi} \arctan \frac{x - d_s/2}{w_s} - \frac{\sqrt{3}b}{6\pi} \arctan \frac{x + d_s/2}{w_s}. \quad (6b)$$

where $u_x(x)$ and $u_z(x)$ describe the edge and the screw displacements, respectively. Here $d_{e,1} = d_{e,2} = d_e/2$, $d_{s,1} = d_{s,2} = d_s/2$, $w_{e,1} = w_{e,2} = w_e$ and $w_{s,1} = w_{s,2} = w_s$. The weights $A_1 = A_2 = \frac{b}{2\pi}$, $B_1 = -B_2 = \frac{\sqrt{3}b}{6\pi}$. In the expression of Eq. 3, the distance $r_{e,12} = d_e$ applies for edge components and $r_{s,12} = d_s$ for screw components. The solution of $\vec{u}$ is illustrated in Figure 1. The two partial dislocations are separated by 7 times of the Burgers vector, which is characterized by the peaks and valley of the misfit density functions ρ_x and ρ_z . A detailed discussion is referred to [7].

2.1. Five-energy-point Method

Up to now we have not discussed how to calculate the gamma surface γ in the framework of Peierls-Nabarro model. In the two-dimensional case, it can be accurately calculated by applying a dense mesh in the faulted plane within a minimum period of area [26, 7]. This is computationally expensive and unnecessary in some case. We test the convergence of Peierls stress with the cutoff of employed plane waves k in describing the basal-plane gamma surface in Mg (see Figure 2) and found that only five data points are required to obtain a reliable Peierls

stress. The expression of five-energy-point gamma surface is

$$\begin{aligned} \gamma_{5\text{-point}}(u_x, u_z) = & R_0 \\ & + R_1 \left\{ \cos(2\pi(\frac{u_x}{a} - \frac{u_z}{\sqrt{3}a})) + \cos(2\pi(\frac{u_x}{a} + \frac{u_z}{\sqrt{3}a})) + \cos(4\pi\frac{u_z}{\sqrt{3}a}) \right\} \\ & + R_2 \left\{ \cos(2\pi(\frac{u_x}{a} - \frac{3u_z}{\sqrt{3}a})) + \cos(2\pi(\frac{u_x}{a} + \frac{3u_z}{\sqrt{3}a})) + \cos(4\pi\frac{u_x}{a}) \right\} \\ & + R_3 \left\{ \cos(4\pi(\frac{u_x}{a} + \frac{u_z}{\sqrt{3}a})) + \cos(4\pi(\frac{u_x}{a} - \frac{u_z}{\sqrt{3}a})) + \cos(8\pi\frac{u_z}{\sqrt{3}a}) \right\} \\ & + I_1 \left\{ \sin(2\pi(\frac{u_x}{a} - \frac{u_z}{\sqrt{3}a})) - \sin(2\pi(\frac{u_x}{a} + \frac{u_z}{\sqrt{3}a})) + \sin(4\pi\frac{u_z}{\sqrt{3}a}) \right\} \\ & + I_2 \left\{ \sin(4\pi(\frac{u_x}{a} - \frac{u_z}{\sqrt{3}a})) - \sin(4\pi(\frac{u_x}{a} + \frac{u_z}{\sqrt{3}a})) + \sin(8\pi\frac{u_z}{\sqrt{3}a}) \right\} \end{aligned} \quad (7)$$

where a is the lattice parameter, and R_i ($i = 0, \dots, 3$), I_i ($i = 1, 2$) are coefficients to be determined. In the expression one group of sin-type functions (I_3) and all the rest terms (i.e., the higher frequency terms) are dropped since their coefficients are ignorable ($< 10^{-2} \text{ mJm}^{-2}$ in Mg, for example). In Eq.7 there are six coefficients that needs to be determined. In principle, if six data points on the gamma surface are known, we can determine the coefficients by solving a group of equations. By default, the gamma surface always goes through zero point, i.e., $\gamma(0, 0) = 0$, so we only need five data points in total.

This expression is applicable for basal dislocations in all hcp crystals and dislocations on the $\{111\}$ plane in all fcc crystals. The Peierls stress in Mg is very low (i.e., 0.5-0.8 MPa [28, 29, 30]), so it requires a very accurate gamma surface as input of the model. If the information of interest is the dislocation core, less terms than five are enough [7]. Also for dislocations with large Peierls stress the requirement of gamma-surface accuracy may also lower down.

As an example, we study the $\{111\}_{\frac{1}{2}}(1\bar{1}0)$ in FeNiCoCrMn high-entropy alloy. Even though the $\{111\}$ stacking is different from $\{0001\}$, their in-plane symmetric operations are same. Therefore our symmetrized-plane-wave expression for gamma surface (Eq.7) applies to this dislocation in the high-entropy alloy. We take only two energy-points (i.e., the intrinsic and globally unstable stacking fault energies γ_{isf} and γ_{us} from [27]) as input of our model. Inserting the two stacking fault energies into Eq. 7, we have $R_0 = 69 \text{ mJm}^{-2}$, $R_1 = 33 \text{ mJm}^{-2}$ and $I_1 = -24 \text{ mJm}^{-2}$. With trial solution in the form of Eq. 6 we determine the values for all the involved parameters (see Table 2). The dislocation core of the high-entropy alloy described by these parameters are shown in Figure 3. Due to the existence of the stable stacking fault and its low energy, the dislocation dissociates into two Shockley partial dislocations. Interestingly, the stacking fault width of about $3b$ is only half of that of the I_1 stacking fault in Mg even though its stacking fault energy is only half of the latter. Based on the dislocation core structure the Peierls stress is computed to be 168.4 MPa, which is in good agreement with experimentally measured Peierls stress $175 \pm 5 \text{ MPa}$ and previously predicted one 178 MPa also using Peierls-Nabarro model [27].

For dislocations that do not dissociate, one-dimensional GSFE curves supply sufficient information for γ . In this case

Figure 3: The two components (u_x, u_z) of the misfit function of $\{111\}_{\frac{1}{2}}(1\bar{1}0)$ dislocation in CrFeCoNiMn high entropy alloy and their derivatives (ρ_x, ρ_z). The dislocation is placed in a coordinate as shown in the inset, i.e., the dislocation line runs along z axis, and the slip plane is xz plane. The z axis is perpendicular to the paper.

the GSFE curve is the minimum energy path on the gamma surface, and the left part of the gamma surface will not be accessed even though a full gamma surface is available. Such an example for the prismatic dislocation in Mg can be found in [31].

3. Particle Swarm Optimization

The algorithm of Particle Swarm Optimization (PSO) simulates the social behaviors of organisms, e.g., fishes, bees, birds, etc [23, 24, 25]. In our everyday life we have such an impression that a swarm of bees can always find their flower source. Suppose each bee represents a possible solution (i.e. a particle in solution space), the flower source represents then the globally optimal solution. In principle, given enough time the particles can always find a locally or the globally optimized solution. The probability to find the global one becomes higher by increasing the size of the swarm. During the time to the flower source, bees have a globally consistent behavior, so they must communicate and exchange their "feeling" for the direction of the flower source. This group behavior can effectively avoid bees to fly in wrong directions (local minima in solution space).

The past decade has seen a quick development of PSO and different variants of the original algorithm have emerged [32]. The details of the PSO algorithm employed in this study are described in Table 3. Each particle i of a swarm of size N is a point in the multidimensional position space (characterized by dimension number n). Initially the position of each particle is assigned random numbers within the safe bounds (b_{lo}, b_{up}) that covers the globally optimal solution. In the following steps, a particle is led by its own "feeling" of the optimal solution (i.e. its current local best position) and also by the that of the group (i.e. the current global best position) through communication. Therefore, the local and global best positions need to be computed at initial and the following time step. At the first

Table 2: The values of input and output parameters for our Peierls-Nabarro modeling of $\{111\}\frac{1}{2}\langle 1\bar{1}0\rangle$ dislocation in FeNiCoCrMn high-entropy alloy. The calculated Peierls stress by us and previous experimental and theoretical results [27] are listed as well. In our calculation the Poisson ratio $\nu = 0.3$.

Material	$a_0(\text{\AA})$	Burger vector $\vec{b}$	$K_e(\text{GPa})$	$\gamma_{us}(\text{mJm}^{-2})$	$\gamma_{isf}(\text{mJm}^{-2})$	τ_p (MPa) (previous)
FeNiCoCrMn	3.59 [27]	$\frac{\sqrt{2}}{2}a_0\langle 110\rangle$	84 [27]	192 [27]	17 [27]	175 $\pm$ 5 [27](Experiment, 77K), 178 [27](Theory, 0K)
$A_1(=A_2)$	$B_1(=-B_2)$	d_e/b	d_s/b	w_e/b	w_s/b	τ_p (MPa) (this study, 0K)
0.5	1.0	3.12	2.94	0.31	0.36	168.4

time step, the initial positions are also their best local positions. By comparing these initial positions we can find the initial best global position. The initial velocity of each particle is also assigned as a random number in the range $U(-|b_{\text{up}}-b_{\text{lo}}|, |b_{\text{up}}-b_{\text{lo}}|)$ or a subset of it.

At the next time step, the initial velocities $v_{i,d}$ are updated firstly by

$$v_{i,d} \leftarrow \omega v_{i,d} + \phi_p r_p (p_{i,d} - x_{i,d}) + \phi_g r_g (g_d - x_{i,d}) \quad (8)$$

where $x_{i,d}$ is the d^{th} dimension of the i^{th} particle, g and p are the global and local best positions. The second term on the right represents the particle is guided by its own sense and the third term describes the particle is affected by its surrounding particles through communication. The weight parameters ϕ_p and ϕ_g determine how the particles' velocities are affected by their local and global "feelings". To increase the randomness in updating velocities, two random numbers r_p and r_g are introduced. The constant ω can be optimized to improve the efficiency of the algorithm. An optimized ω is close to 1 and 1 is a good choice in most of the case. With updated velocities the new positions are calculated by $x_i \leftarrow x_i + v_i$. At the new position the value of aim function for each particle is then calculated and compared with that of its old position. Accept the new position if the new local best position is in the wanted direction, i.e., a_{245} direction close to the gradient of the aim function. The last step is to update the global best position in the same procedure as in the initial time step. The velocities are updated using Eq.8. These steps are iterated until the value of the aim function meets the termination criterion.

Since the time-consuming part of the algorithm (line 8-20 in Table 3) consists of two for-loops, such a structure is particularly suitable to be parallelized. Inside this part computing the values of aim function f can also be computationally expensive, which is exactly the case for the calculation of E_c in Peierls-Nabarro model. Fortunately this procedure also consists of a for-loop that is not difficult to be parallelized. It is worth to notice that the PSO requires the particles to exchange their "feelings" for the optimal solution, so an ideal scaling of speedup is not expected.

4. Scaling and Performance

The algorithm of PSO is implemented in C++ language on the GenuineIntel machine of "CMMC" cluster of Max-Planck-Institut für Eisenforschung GmbH. The cluster consists of 650 nodes and for each node there are 20 shared-memory cores. As an initial test, we parallelize the algorithm using OpenMP library for shared-memory cores. As an example, we use the

Table 3: (Algorithm 2) The Algorithm of Particle Swarm Optimization. It is readily used to solve the Peierls-Nabarro equation when the aim function $f \leftarrow E_c$ and a particle's position $p_i \leftarrow (w_i, A_i, B_i, r_{ij})$.

1:	for each particle $i = 1, \dots, N$ do
2:	initialize the particle's position with a uniformly distributed random vector: $x_i \sim U(b_{\text{lo}}, b_{\text{up}})$
3:	initialize the particle's best known position to its initial position: $p_i \leftarrow x_i$
4:	if $f(p_i) < f(g)$ then
5:	update the swarm's best known position: $g \leftarrow p_i$
6:	initialize the particle's velocity: $v_i \sim U(- b_{\text{up}} - b_{\text{lo}} , b_{\text{up}} - b_{\text{lo}})$
7:	end for
8:	while a termination criterion is not met do:
9:	for each particle $i = 1, \dots, N$ do
10:	for each dimension $d = 1, \dots, n$ do
11:	pick random numbers: $r_p, r_g \sim U(0, 1)$
12:	update the particle's velocity: $v_{i,d} \leftarrow \omega v_{i,d} + \phi_p r_p (p_{i,d} - x_{i,d}) + \phi_g r_g (g_d - x_{i,d})$
13:	update the particle's position: $x_i \leftarrow x_i + v_i$
14:	if $f(x_i) < f(p_i)$ then
15:	update the particle's best known position: $p_i \leftarrow x_i$
16:	if $f(p_i) < f(g)$ then
17:	update the swarm's best known position: $g \leftarrow p_i$
18:	end for
19:	end for
20:	end while

algorithm to solve the Peierls-Nabarro equation to obtain the core structure of $\{10\bar{1}0\}\langle 11\bar{2}0\rangle$ dislocation. We test for 30, 300 and 3000 particles and 1000, 10000 and 100000 iteration steps.

The Performance of the parallelized algorithm is shown in Figure 4 (a). The best performance is obtained for 3000 particles and 100000 iteration steps, i.e., 77.5%. The Speedup scales linearly with the number of cores, which demonstrates that the PSO is very suitable for future massive parallelization.

Figure 4 (b) shows the performance is also affected by problem size/workload, i.e., the numbers of iteration steps and particles in this case. In order to separately check how the speedup changes with the number of iteration step and particle size, we keep one of them as a constant. The performance of the tests is obtained with 20 cores. When the number of iteration step is 10000, the speedup increases from 10.5 to 15.5 with more particles; when the particle size is 300, the speedup changes from 12.2 to 15.4 with more iteration steps. However, the gain with heavier workload converges quickly with the numbers of particles and iteration steps. For example, when the number of particles increases 10 times from 300 to 3000, the speedup changes only from 15 to 15.5. The underlying reason lies in the principle of parallelization, which is summarized in Amdahl's law. Amdahl's law can be formulated as the speedup $S = \frac{1}{1-p+p/N}$, where p is the parallelable part of a job, N is the number of cores applied in one simulation. According to the law, the ac-

Figure 4: The performance of our accelerated Particle Swarm Algorithm (PSA). (a) The speedups of different problem sizes increase with applied core number. (b) The speedups with 20 cores increase with problem sizes (number of particles or iteration steps).

celeration is gained by distributing the parallelable part of one job to multiple cores and computing them in a parallel manner. Since there is always serial part of one task ($p < 1$), the best performance S_{max} is not N but $\frac{1}{1-p}$. The law also clearly shows that the performance can be enhanced by increasing the parallelable workload, as we have done in the tests.

With the parallelized algorithm of PSO we can solve the Peierls-Nabarro equation within several minutes for dislocations in conventional alloys. Since there are usually more than five components in high-entropy alloys, it is expected there exist more local minima in the search space for solutions. Therefore, for dislocations in high-entropy alloys more particles and iteration steps are probably required to solve the equation, which means a higher computational cost and longer run time. In this case our parallelized algorithm is particularly useful in reducing the run time and increasing the efficiency of solving

the Peierls-Nabarro model.

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