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# Atomistic to continuum mechanics description of crystal defects with dislocation density fields: application to dislocations and grain boundaries

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## Abstract

The atomic structure of crystal defects such as dislocations, grain or phase boundaries, control these defects' properties: their mobility, ability to cross-slip, or solute segregation. These crystal defects can be conveniently studied by atomistic simulations and one then needs to transfer relevant information at the upper scale to model microstructures containing a large number of defects, e.g., a polycrystal. Here, we propose an atomistic to continuum mechanics crossover method that (i) represents the atomic structure of dislocations cores by an appropriate Nye dislocation density tensor field and (ii), captures quantitatively the short and long range mechanical fields of defects. For (i), we propose a modified and improved interpolation method based on the original work by Hartley and Mishin. For (ii), we use a field dislocation mechanics framework that rigorously calculates / evaluates the mechanical fields associated with any Nye dislocation density distribution. The transfer method relies on molecular static calculations using two energetic models - ab-initio for screw dislocation core simulations in tungsten, and EAM potential for low and large angle grain boundaries in copper. Our findings demonstrate the effectiveness of the proposed approach in reconstructing the Burgers vector, and continuous strain and rotation fields. The framework is further applied to analyze the elastic interactions between extrinsic edge dislocations and a low angle grain boundary in copper.

*Keywords:* dislocations, grain boundaries, Nye tensor, Ab-Initio, Molecular Statics, Field Dislocation Mechanics.

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## 1. Introduction

1 Crystal defects, in particular dislocations and grain boundaries (GBs), are well known to control the mechanical  
2 properties of crystalline materials. A thorough understanding of these defects is essential for designing materials with  
3 mechanical properties tailored for a wide range of applications [1]. Dislocation and GB physics is a multidisciplinary  
4 field that investigates the behavior and properties of defects across a broad spectrum of scales, from the atomic-level  
5 where, for instance, the dislocation core involves a few atoms only, up to the scale of polycrystals where billions of  
6 dislocation lines interact with each others and with GBs. At the atomic scale, Molecular Dynamics/Statics (MD/MS)  
7 simulations are widely used to model the fundamental structures and properties of dislocations or GBs. These simu-  
8 lations provide detailed and quantitative insights on defected atomic configurations, energies, mobilities, etc. [2, 3].  
9 They are also widely used to predict the interactions between dislocations and grain boundaries, and discern con-  
10 figurations that facilitate dislocation absorption or transmission through grain boundaries in metallic materials [4].  
11 Nonetheless, atomistic simulations are usually limited to small time and size scales, typically of the order of few  
12 nanoseconds and tens of nanometers. As such, multiscale efforts are needed to extract relevant physical and mechani-  
13 cal information from atomistic simulations, and incorporate it in larger scale models, in order to simulate realistic and  
14 statistically meaningful microstructures. Such larger scale modelling approaches are discrete dislocation dynamics

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15 [5], phase field models [6], or continuum mechanics based crystal defect models [7].

16  
17 Continuum mechanics approaches are well suited for tracking the evolution of mechanical fields and defected  
18 microstructures (elastic/plastic deformation, internal stresses, dislocation densities etc.) at the mesoscale, i.e., at the  
19 scale of grains. Frank and Bilby were pioneers in the development of such fundamental theories for mechanically  
20 representing the structure of grain and phase boundaries [8, 9]. The continuous approach they proposed describes the  
21 interface as a dislocation surface density, more precisely by a Burgers vector density, that accommodates the incom-  
22 patibility of elastic transformation at the interface [9]. This model was later adopted by Read and Shockley to establish  
23 a correlation between the excess energy of GBs and their misorientation angle [10]. Recently, this model has seen  
24 extensions to more general grain boundaries. It was shown that a link between misorientation, Burgers vector content  
25 of grain boundaries, and GB excess energy, can be established for a broad spectrum of misorientations and GB types  
26 using a generalized Read and Shockley model [11]. The Frank and Bilby model has also been successfully applied to  
27 investigate the migration of tilt GBs in a mean-field micromechanical framework [12]. In a similar context, phase field  
28 approaches have demonstrated their ability to study various aspects of crystal elasticity [13], dislocation mobility [14],  
29 and deformation twinning in crystalline materials [15]. Phase field models can be enriched by incorporating informa-  
30 tion from atomistic simulations. For instance, stacking fault energies as obtained from density functional theory (DFT)  
31 calculations can be introduced, which allows to model the dissociated structures and mobility of dislocation cores [16].

32  
33 The field dislocation mechanics (FDM) model considered in the present work is a somewhat alternative to disloca-  
34 tion phase field models at small scales [17]. This approach provides a continuous representation of dislocation cores  
35 using an appropriate distribution of dislocation density. It relies on the Nye dislocation density tensor [18], the Kröner  
36 incompatibility equation [19], and the dislocation density transport equation [20]. One of the primary advantages of  
37 this model is its ability to provide a fully continuous description of crystalline defects using Nye dislocation densities,  
38 which enables to model dislocation core structures [21]. The presence of a Nye dislocation density is linked to an  
39 incompatible elastic distortion and generates internal stresses. Although the FDM approach can be applied to disloca-  
40 tions and grain boundaries, the introduction of disclination fields [22] was proposed to offer an alternative description  
41 of such grain boundaries. This model has been successfully applied to tilt GBs [23] and twist interfaces [24]. It  
42 notably enables the reproduction of structural units that compose grain boundaries, their excess energy [25] and their  
43 migration kinematics [26]. Disclination and/or dislocation density approaches thus allow for the substitution of the  
44 atomic structure of defects (such as dislocations and interfaces) for an equivalent representation using defect densities,  
45 thereby enabling their incorporation into a continuum mechanics framework for upscaling.

46  
47 Based on the framework presented above, we have developed a novel method for an atomistic to continuum me-  
48 chanics crossover with the objective of capturing the core structure and the continuous mechanical fields of various  
49 crystal defects, including dislocations and grain boundaries. We restrict ourselves to field dislocation mechanics here,  
50 but the approach can be extended to incorporate disclination fields. Our approach thus involves the description of  
51 the atomic structure of crystal defect cores in terms of an equivalent Nye dislocation density. The first stage entails  
52 computing the per-atom elastic distortion field from atomistic simulations, the incompatible part of which yields the  
53 associated Nye dislocation density. For this task, we are using the Hartley Mishin algorithm [27] that provides the  
54 inverse elastic transformation (also called correspondence tensor) as well as the Nye density on each atom in an  
55 atomistic configuration. For the second stage, we explore the appropriate metrics, whether it be the per-atom inverse  
56 elastic transformation or directly the per-atom Nye tensor, to perform our transition from atomistic data to our contin-  
57 uum mechanics FDM model. More precisely, as our FDM model field equations are numerically approximated on a  
58 regular fast Fourier transform (FFT) grid, we try different interpolations of atomistic data (transformation or Nye ten-  
59 sors) onto the FFT grid and compare with atomistic data in terms of Burgers vector and short/long range mechanical  
60 fields (elastic strains and rotations). We assess our atomistic to continuum mechanics crossover by the ability of the  
61 atomistic-aided FDM to predict the elastic fields of different defects. Defects include screw dislocations dipoles, edge  
62 dislocations array and structural units in high angle tilt grain boundaries.

63  
64 The structure of this paper can be summarized as follows. First, we provide an initial overview of the atomistic  
65 methods employed for simulating crystal defects (Section 2). This includes Density Functional Theory (DFT) methods  
66 to model  $1/2[111]$  screw dislocation dipoles in tungsten and Molecular Statics (MS) for producing high and low-angle

67 tilt grain boundaries in copper. Following this, a brief overview of dislocation mechanics allows us to introduce the  
 68 Hartley and Mishin algorithm used to compute the per-atom lattice correspondence and Nye tensors. The latter part  
 69 of Section 2 is devoted to elucidating the method employed for transitioning from atomistic data to our continuous  
 70 mechanical model. Section 3 is dedicated to applications of the crossover method, where we systematically assess the  
 71 ability of FDM to reproduce the Burgers vector of defects and their mechanical fields. The final part of Section 3 is  
 72 focused on applying the transfer method to investigate the interactions between extrinsic edge dislocations and a low  
 73 angle tilt grain boundary. Section 4 concludes our study and presents further directions.

## 74 2. Methods

### 75 2.1. Numerical simulation methods

#### 76 2.1.1. Atomistic approaches

77 Ab-initio calculations based on the density functional theory (DFT) were performed to simulate the core structure  
 78 of  $1/2[111]$  screw dislocations in body-centered cubic (BCC) tungsten. All computations were carried out using  
 79 the Vienna ab-initio simulation package (VASP) [28]. The exchange-correlation interactions were described using  
 80 the Generalized Gradient Approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) parametrization. A screw  
 81 dislocation dipole is inserted within a supercell containing 135 atoms with three-dimensional (3D) periodic boundary  
 82 conditions using periodicity vectors  $\vec{C}_1 = 5/2[1\bar{2}1] + 9/2[\bar{1}01]$ ,  $\vec{C}_2 = 5/2[1\bar{2}1] - 9/2[\bar{1}01]$ , and  $\vec{C}_3 = 1/2[111] = \vec{b}$   
 83 as presented in the recent work of Bienvenu et al. [29][30][31] (See Figure S1 in Supplementary Material). We set  
 84 a kinetic energy cutoff of 400 eV for the plane-wave basis and convergence criterion of 0.05 eV/Å on the forces for  
 85 ionic relaxations.

86  
 87 To simulate symmetric tilt GBs in face-centered cubic (FCC) copper, we employed the Molecular Dynamics  
 88 LAMMPS code [32]. The atomic interactions were modeled using the embedded atom method (EAM) potential of  
 89 Mishin et al [33] for Cu. This potential accurately predicts key physical properties of Cu, including the lattice pa-  
 90 rameter, cohesive energy, vacancy formation energy, GB excess energies and elastic stiffness moduli. In this study,  
 91 we consider the low-angle grain boundary (LAGB)  $\Sigma 365(27\bar{1}0)[001]$  and the high-angle grain boundary (HAGB)  
 92  $\Sigma 5(310)[100]$ . Figure S2 (supplementary material) illustrates the simulation boxes for each of these GBs. Note that  
 93 each computational cell contains two opposite grain boundaries because of periodic boundary conditions. The simu-  
 94 lation cell dimensions for LAGB and HAGB are  $(137 \times 252 \times 3.615 \text{ \AA}^3)$  and  $(293 \times 391 \times 3.615 \text{ \AA}^3)$ , respectively. These  
 95 dimensions are sufficiently large to prevent any significant interaction between the two opposite grain boundaries.  
 96 Molecular Statics (MS) calculations were performed to determine the minimum energy configuration of each grain  
 97 boundary. The standard simulation methodology includes rigid body translation of rotated grains, application of atom  
 98 deletion criteria and the use of the conjugate gradient method for relaxing the initial atomic structures. The details of  
 99 this methodology were extensively described by Tschopp et al. [34].

#### 100 2.1.2. Continuum mechanics approach: Field Dislocation Mechanics

101 We provide here a brief overview of the FDM model with the most important equations, more details about the  
 102 model can be found in reference [17]. We consider the elastic deformation of a body containing dislocation lines. The  
 103 presence of dislocations will be the source of elastic deformation and internal stresses. We first consider a general fi-  
 104 nite deformation setting and we then simplify into a small strain approximation. For simplicity, let us consider a body  
 105 containing one dislocation line. The model begins by relating the incompatibility of the elastic transformation tensor  
 106 to the Burgers vector. Let us consider two material configurations denoted as the reference configuration and the de-  
 107 formed configuration, distinguished by their position vectors  $\mathbf{X}$  and  $\mathbf{x}$ , respectively. The reference system corresponds  
 108 to a continuous crystal (without cracks or voids) and without deformation. The deformed material configuration is  
 109 obtained by applying to the reference configuration the transformation  $\mathbf{F} = \partial \mathbf{x} / \partial \mathbf{X}$ . The deformation gradient tensor  $\mathbf{F}$   
 110 is multiplicatively decomposed into plastic  $\mathbf{F}_p$  and an elastic  $\mathbf{F}_e$  tensors,  $\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p$ . Both tensors contain an incom-  
 111 patible non-gradient part, reflecting the elastic and plastic discontinuity due to a non-zero Burgers vector. A possible  
 112 measure of this incompatibility is precisely the Burgers vector [35]. The Burgers vector  $\mathbf{b}$  is defined as the integral of  
 113  $\mathbf{F}_e^{-1}$  along a closed circuit ( $C$ ) around the dislocation line and is written as follows:

$$\mathbf{b} = - \oint_C \mathbf{F}_e^{-1} \cdot d\mathbf{x}. \quad (1)$$

114 In the above equation, the Burgers vector is measured in the intermediate, or plastic, configuration. If  $\mathbf{b}$  equals  
 115 zero, it indicates compatibility of the elastic deformation. Conversely, when  $\mathbf{b}$  is non-zero, there is incompatibility.  
 116 By applying Stokes' theorem to equation (1), we derive:

$$\mathbf{b} = - \iint_S \mathbf{curl}(\mathbf{F}_e^{-1}) \cdot \mathbf{n} dS, \quad (2)$$

117 where  $S$  is the surface, with the unit normal  $\mathbf{n}$ , bounded by the Burgers circuit. From another point of view now,  
 118 the Burgers vectors can be geometrically described through a second-order tensor known as the dislocation density  
 119 tensor or so-called Nye tensor  $\alpha$  defined as [18]:

$$\mathbf{b} = \iint_S \alpha \cdot \mathbf{n} dS. \quad (3)$$

120 The tensor  $\alpha$  has components  $\alpha_{ij} = b_i t_j$  in the Cartesian coordinate system, where the density  $b_i$  is the length  
 121 of Burgers vector in direction  $i$  per unit surface and  $t_j$  is the unit dislocation line vector component in direction  $j$ .  
 122 This means that the diagonal terms of the Nye tensor  $\alpha$  represent screw dislocations whereas the non-diagonal terms  
 123 represents edge dislocations. By identifying the two equations above, we obtain a non-integral expression that relates  
 124 the inverse elastic transformation tensor to the Nye tensor:

$$\alpha = -\mathbf{curl}(\mathbf{F}_e^{-1}). \quad (4)$$

125 In a small strain framework now, the inverse of the elastic transformation tensor  $\mathbf{F}_e^{-1}$  is related to the elastic  
 126 distortion  $\mathbf{U}_e$  by  $\mathbf{F}_e^{-1} = \mathbf{I} - \mathbf{U}_e^e$ , where  $\mathbf{I}$  is the second-order identity tensor. The equation (4) can be rewritten as:

$$\alpha = \mathbf{curl}(\mathbf{U}_e). \quad (5)$$

127 Following the work By Acharya [], we decompose the elastic distortion into an incompatible non-gradient, curl  
 128 part  $\mathbf{U}_e^\perp$ , and a compatible, curl-free part  $\mathbf{U}_e^\parallel$ , which is a gradient. We therefore apply the Stokes Helmholtz decompo-  
 129 sition:

$$\mathbf{U}_e = \mathbf{U}_e^\perp + \mathbf{U}_e^\parallel = \mathbf{curl}\chi + \mathbf{grad}\mathbf{w}. \quad (6)$$

130 By applying the  $\mathbf{curl}$  operator to equation (6), we extract the incompatible elastic distortion, such that we have:

$$\alpha = \mathbf{curl}(\mathbf{U}_e^\perp). \quad (7)$$

131 To obtain a unique and purely rotational solution to the above equation, we must also satisfy  $\mathbf{div} \mathbf{U}_e^\perp = 0$ . By using  
 132 the identity  $\mathbf{curl}(\mathbf{curl} \mathbf{A}) = \mathbf{grad}(\mathbf{div} \mathbf{A}) - \mathbf{div}(\mathbf{grad} \mathbf{A})$ , the incompatible elastic distortion is given as the solution of  
 133 the following Poisson-type equation:

$$\mathbf{div}(\mathbf{grad} \mathbf{U}_e^\perp) = \Delta \mathbf{U}_e^\perp = -\mathbf{curl}(\alpha). \quad (8)$$

134 Equation (8) is solved through a computationally efficient numerical spectral method based on fast Fourier trans-  
 135 form (FFT) algorithms, as detailed by Djaka et al. [36]. In order to know the total elastic distortion, we need to  
 136 determine the compatible part, which serves to satisfy the stress equilibrium. Let us call  $\mathbf{T}$  the symmetric Cauchy  
 137 stress tensor and  $\mathbf{C}$  the fourth order elasticity tensor. In the present study, we will use the elastic moduli obtained  
 138 from Ab-initio simulations for the screw dislocation in tungsten, whereas for the GBs in copper, we employ the elastic  
 139 constants predicted by the Mishin EAM potential [33]. The elastic constants were calculated in the standard basis of  
 140 the BCC and FCC structures (see table (1)). The stress tensor reads:

$$\mathbf{T} = \mathbf{C} : \mathbf{U}_e = \mathbf{C} : (\mathbf{U}_e^\perp + \mathbf{U}_e^\parallel). \quad (9)$$

Table 1: Elastic properties predicted for Tungsten with our DFT calculations and via EAM potential for copper. The elastic constants in tungsten were computed within a cell with 1 atom using a  $34 \times 34 \times 34$  k-point mesh .

	$C_{11}$ (GPa)	$C_{12}$ (GPa)	$C_{44}$ (GPa)
Tungsten	514.46	203.91	142.4
Copper	169.9	122.6	76.2

141 and must satisfy the equilibrium equation  $\mathbf{div} \mathbf{T} = 0$  in the absence of inertia effects. Finally, using the definition  
 142 of  $\mathbf{U}_e$  in equation (6), the stress equilibrium equation can be rewritten as:

$$\mathbf{div} (\mathbf{C} : \mathbf{grad} \mathbf{w}) + \mathbf{f}^\perp = 0, \quad (10)$$

143 where  $\mathbf{f}^\perp = \mathbf{div}(\mathbf{C}:\mathbf{U}_e^\perp)$  can be interpreted as a volumetric force resulting from the elastic incompatibility associated  
 144 with dislocations. The equation (10) is also approximated through a computationally efficient scheme based on FFT  
 145 algorithms in the framework of heterogeneous elasticity [36].

## 146 2.2. Atomistic to continuum mechanics transfer methods

### 147 2.2.1. Hartley and Mishin original algorithm

148 In this section, we adopt the approach introduced by Hartley and Mishin [27] to calculate the Nye tensor  $\alpha$  per  
 149 atom. The Nye tensor can be expressed as the curl of lattice correspondence tensor  $\mathbf{G}$ , which is the inverse elastic  
 150 transformation that maps the position vectors of atoms in a deformed crystal configuration  $\mathbf{dx}$  onto those of a perfect  
 151 reference crystal configuration  $\mathbf{dX}$  by the equation:

$$\mathbf{dX} = \mathbf{G}.\mathbf{dx}. \quad (11)$$

152 To compute the lattice correspondence tensor  $\mathbf{G}$ , we define  $\mathbf{P}^\gamma (\gamma = \{1, 2, 3, \dots, n\})$  and  $\mathbf{Q}^\beta (\beta = \{1, 2, 3, \dots, m\})$  as the  
 153 set of position vectors between atom  $i$  and all its neighboring atoms ( $n$  and  $m$ ) within a specified cutoff radius  $R_c$  in  
 154 the perfect configuration and the deformed configuration respectively. It is important to note that the choice of cutoff  
 155 radius significantly impacts the  $\mathbf{G}$  fields and the Burgers vector calculations. In the systems simulated here, we select a  
 156 cutoff distance of  $R_c = 0.93a_0$  and  $0.86a_0$  for BCC and FCC, respectively. These values correspond to half the distance  
 157 between the first and second neighbor shells in the BCC and FCC systems. For each  $\mathbf{Q}^\beta$  we locate the corresponding  
 158  $\mathbf{P}^\gamma$  with the closest angle match. This is achieved by calculating the angular difference between the two vectors, i.e.,  
 159 for each  $\mathbf{Q}^\beta$  we seek the  $\mathbf{P}^\gamma$  vector yielding the shortest angle. If there is no  $\mathbf{P}^\gamma$  vector found within a fixed tolerance  
 160  $\theta_{max}$ , we exclude that  $\mathbf{Q}^\beta$ . However, if a match is found, we compare the lengths of the two  $\mathbf{Q}^\beta$  vectors and retain the  
 161 one that is closest in length to  $\mathbf{P}^\gamma$ . According to Hartley and Mishin [27] suggestion, we employed  $\theta_{max} = 43^\circ$  for  
 162 BCC and  $\theta_{max} = 27^\circ$  for FCC systems, which closely aligns with half of the angle between the  $\mathbf{P}^\gamma$  vectors. The lattice  
 163 correspondence tensor  $\mathbf{G}$  is evaluated for a given atom as a least squares solution of the linear matrix equation:

$$\mathbf{Q}.\mathbf{G} = \mathbf{P}. \quad (12)$$

164 According to Harley and Mishin convention, the Nye tensor  $\alpha$  can be expressed as function of the lattice corre-  
 165 spondence tensor  $\mathbf{G}$  by:

$$\alpha = -\mathbf{curl}(\mathbf{G}). \quad (13)$$

166 It is important to highlight that within the Hartley and Mishin approach, the counterpart to the lattice correspon-  
 167 dence tensor is represented as the transpose of the elastic transformation inverse in the FDM approach. This means  
 168 that:

$$\mathbf{G} = (\mathbf{F}_e^{-1})^T. \quad (14)$$

169 By using the Einstein notation, the Nye tensor in our FDM model is thus expressed in rectangular cartesian  
 170 components as:

$$\alpha_{ij} = -\epsilon_{jkl} \frac{\partial G_{il}^T}{\partial x_k}, \quad (15)$$

171 where  $\mathbf{e}$  is the Levi-Cevita permutation tensor. In the Hartley and Mishin algorithm, the per-atom Nye tensor is  
 172 then estimated through an approximation of spatial derivatives involved in the curl operation. The algorithm has been  
 173 recently implemented in available atomistic tools designed for the construction and analysis of large-scale atomic  
 174 systems, such as Atomman [37] and Atomsk [38]. Both tools were tested and yielded similar results for the  $\mathbf{G}$  and  $\alpha$   
 175 per-atom fields.

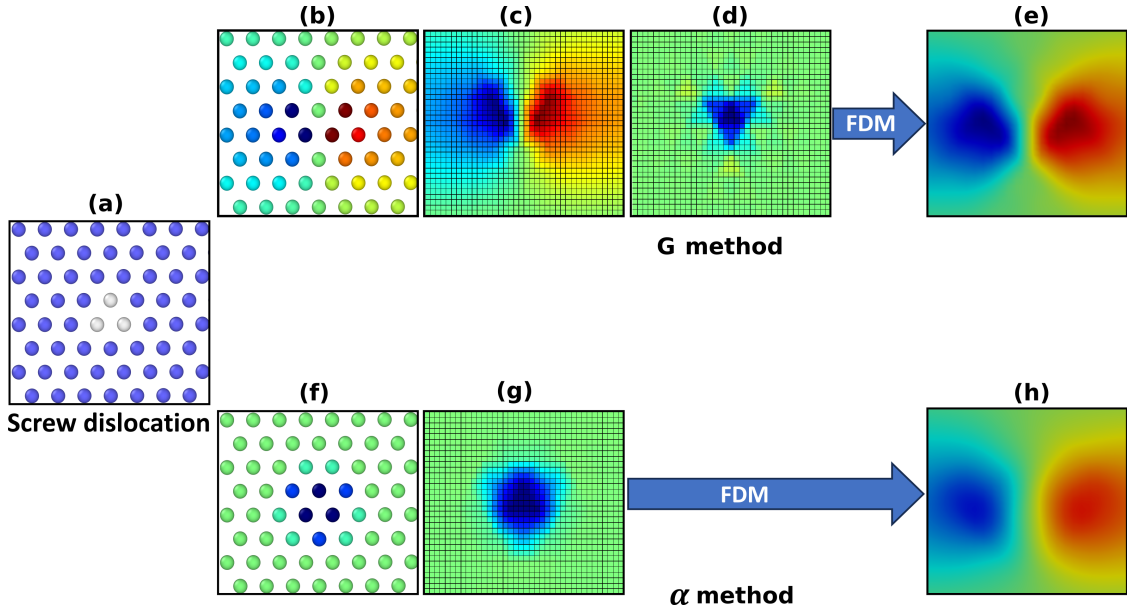


Figure 1: Schematic representation of the atomistic to continuum transfer techniques: (a) Visualization of a  $1/2[111]$  tungsten screw dislocation core in OVITO[39]. The atomistic core structure is colored using common neighbor analysis: Blue atoms represent BCC environment and white atoms indicate a non-BCC environment. The figures (b),(c), (d) and (e) depict the workflow of the G method. (b) The component  $G_{23}$  of the per-atom lattice correspondence tensor calculated by Harley and Mishin algorithm. (c) Interpolation  $G_{23}$  on the FFT grid. (d) Calculation of the component  $\alpha_{33}$  of the Nye tensor on the FFT grid. (e) Visualization of elastic distortion maps obtained from solving the FDM equations. The figures (f),(g) and (h) represent the workflow of the  $\alpha$  method. (f) The component  $\alpha_{33}$  of the per-atom Nye tensor calculated by Harley and Mishin algorithm. (g) Interpolation of  $\alpha_{23}$  on the FFT grid. (h) Visualization of elastic distortion maps obtained from solving the FDM equations.

176

### 177 2.2.2. Atomistic to continuum transfer

178 In this section, we outline two different approaches employed for using possible atomistic data for a given crystal  
 179 defect (dislocations or GBs), as input in the FDM model. We remind that the FDM field equations (8) and (10) are  
 180 numerically approximated on a regular FFT grid, following [36]. As such, we need to transfer per-atom atomistic (ab-  
 181 initio or MS) data onto an FFT grid. Atomistic, per-atom data fields, can be either  $\mathbf{G}$  or directly  $\alpha$ . As illustrated in  
 182 Fig. 1, the first approach, denoted G method, involves the computation of the per-atom lattice correspondence tensor  
 183 using the Hartley and Mishin algorithm (Fig.1b). The tensor components are then interpolated onto the FFT grid  
 184 (Fig.1c), on which we can then estimate the curl to determine the Nye tensor using a finite difference approximation  
 185 (Fig.1d). From this, we can solve the FDM equations to obtain the continuous elastic distortion field Fig.1e. The  
 186 second approach, denoted  $\alpha$  method, involves the calculation of the per-atom Nye tensor using the Hartley and Mishin  
 187 algorithm (Fig.1f). The components  $\alpha_{ij}$  of this tensor are then directly interpolated on the FFT grid (Fig.1g) and use  
 188 as input to solve the FDM equations, leading to another continuous elastic distortion field (Fig.1h). Finally, we can  
 189 compare the continuous elastic distortion fields obtained via both G and  $\alpha$  methods to the elastic per-atom elastic  
 190 fields obtained using the Hartley and Mishin algorithm.

191 **3. Results and discussion**

192 **3.1. Benchmark test**

193 The transfer methods introduced in section 2.2.2 are first assessed by considering  $1/2[111]$  screw dislocations  
 194 in tungsten. Figure 2 depicts the influence of FFT grid resolution on the Nye component  $\alpha_{33}$  distribution using G  
 195 and  $\alpha$  methods. For the finest resolution tested ( $0.5 \text{ \AA}$ , Fig. 2 (b) and (c)), both methods successfully capture the  
 196 screw density distribution obtained with DFT (Fig. 2 (a)). However, the three-fold symmetry of the screw dislocation  
 197 core is only captured by the G method at  $0.5 \text{ \AA}$  resolution (Fig. 2 (b)). It is also with this method and resolution that  
 198 we manage to obtain the most compact core, which is a specific feature of screw dislocation cores in BCC metals.  
 199 Fig. 2 (c) and (e) show that a  $2 \text{ \AA}$  resolution does not reproduce the 3-fold symmetry of the dislocation core, for either  
 200 method. We have quantitatively evaluated both methods by calculating the error on the magnitude of the Burgers  
 201 vector relative to the ideal value ( $b_{ideal} = 2.762 \text{ \AA}$ ). Given the Nye tensor definition in equation (3), the Burgers vector  
 202 is numerically calculated by integrating the Nye tensor over a rectangular grid in a plane normal to the dislocation  
 203 line. Figure 2 (f) depicts the variation of the error as a function of the FFT grid resolution for both methods.

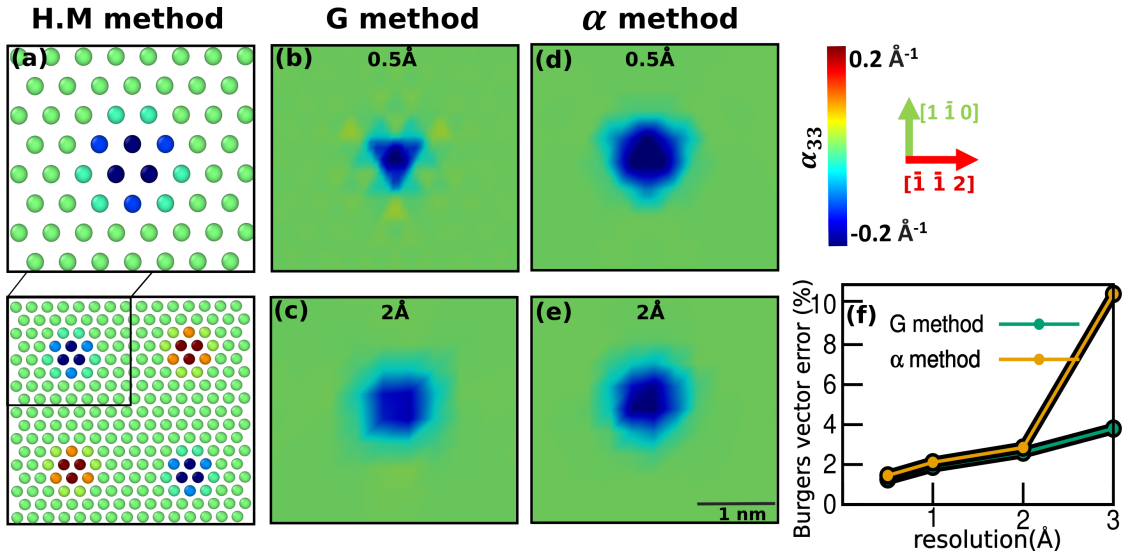


Figure 2: Screw dislocations in tungsten. Effect of FFT grid resolution on Nye dislocation density distributions and Burgers Vector norm error using G and  $\alpha$  methods. (a) Visualization of the per-atom component  $\alpha_{33}$  of the Nye tensor as obtained from the Hartley-Mishin method applied to the DFT calculations. Red represents positive dislocation density and blue the negative one. (b) and (c): maps illustrating the screw dislocation density distribution obtained using the G method with FFT Grid resolutions of  $0.5 \text{ \AA}$  and  $2 \text{ \AA}$ , respectively. (d) and (e) depict screw dislocation density distributions using the  $\alpha$  method with  $0.5 \text{ \AA}$  and  $2 \text{ \AA}$  FFT grid resolutions. (f) The variation of the Burgers vector norm error as a function of the grid resolution using the G method (green line) and  $\alpha$  method (yellow line).

204

205 We observe two distinct regions in Fig. 2 (f). For resolutions up to  $2 \text{ \AA}$ , both methods exhibit similar efficiency,  
 206 while for resolutions higher than  $2 \text{ \AA}$ , the  $\alpha$  method shows noticeable increase in the error percentage. This correlates  
 207 with the fact that the core is less compact than expected for higher resolutions. Thereby, when using coarser reso-  
 208 lutions, the accurate description of the core is compromised due to the loss of information during interpolation. An  
 209 identical procedure was carried out for edge dislocations within LAGB in copper (see Figure S3 in Supplementary  
 210 Material) and also showed an increased error percentage for resolutions higher than  $0.5 \text{ \AA}$ , and a loss of core symme-  
 211 try for resolutions of  $2 \text{ \AA}$  and more. Consequently, in the following, we consider the resolution of  $0.5 \text{ \AA}$ , which provides  
 212 the best description of the dislocation core.



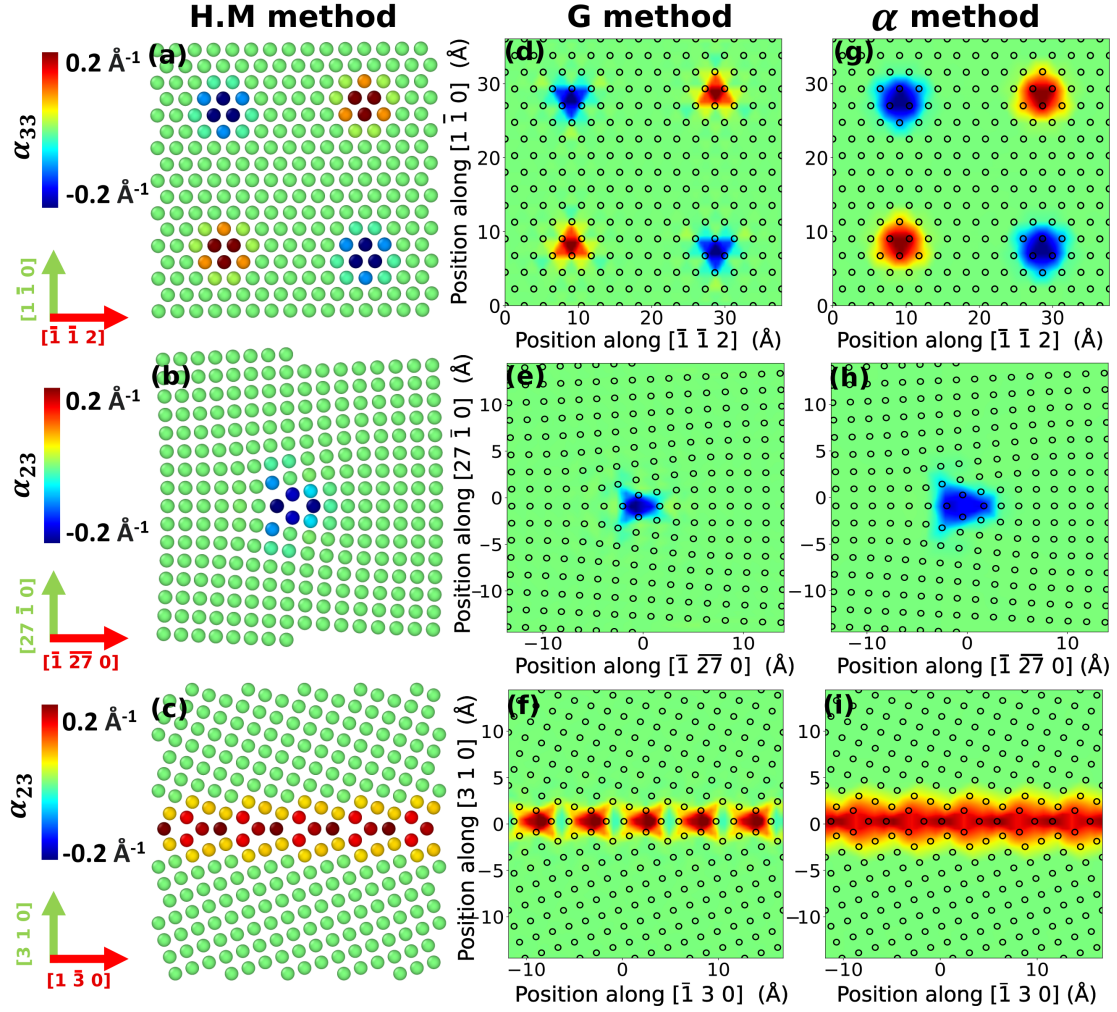


Figure 3: Comparison of Nye dislocation density distributions obtained with the G and  $\alpha$  transfer methods using a 0.5 Å FFT grid resolution. (a), (b) and (c) Visualization of the component  $\alpha_{33}$  and  $\alpha_{23}$  of the Nye tensor for the screw dislocation quadruple in tungsten, structural units within LAGB and HAGB in copper respectively after atomistic relaxation. (d), (e) and (f) Represent maps displaying the screw and edge dislocation densities obtained via the G method. (g), (h) and (i) show the same densities obtained with the  $\alpha$  method.

### 213 3.2. Inspection of Nye dislocation density distributions

214

215 In the following, we compare qualitatively the efficiency of the G and the  $\alpha$  methods in terms of Nye dislocation  
 216 density distributions for the  $1/2[1\ 1\ 1]$  screw dislocations in tungsten (screw densities), LAGB and HAGB in copper  
 217 (edge densities). The first column of Figure 3 shows the distribution of the atomic Nye tensor for the three defects  
 218 studied. Hartley and Mishin's method can be extended to calculate the Nye tensor within a grain boundary. This is  
 219 particularly useful because identifying the ideal reference configuration can be challenging for systems as complex as  
 220 grain boundaries. In this study, we opted for the Displacement Shift Complete (DSC) lattice as our reference system  
 221 for the grain boundary [40], as it is typically closely aligned with the positions of the atoms within the GB [41]. In  
 222 the third row, we examine the atomic Nye tensor of a symmetric tilt HAGB  $\Sigma 5(3\ 1\ 0)[0\ 0\ 1]$  (Figures 3 (c), Fig. 3 (f)  
 223 and Fig. 3 (i)). This specific system holds considerable importance to assess our approach as the GB structure is  
 224 not described by a dislocation array as for LAGB, but by structural units. We observe that for all defects, the G  
 225 method results in a highly concentrated Nye edge dislocation density distribution in each structural unit, whereas

226 the  $\alpha$  method produces a spread-out distribution. Interestingly, the result from the G method for LABG and HAGB  
 227 suggests that each structural unit can be interpreted as an edge dislocation with an equivalent Burgers vector  $[0\ 1\ 0]$ .  
 228 While dislocation based models are usually said to be limited to low misorientations ( $< 15^\circ$ ), our results rather suggest  
 229 they are actually also applicable to HAGBs. Last but not least with the G method, the edge dislocation core in the  
 230 LABG and the structural unit cores in the HAGB have the largest edge dislocation density at the place where there is  
 231 no atom (where there is an excess volume). As such, the G method offers a more appropriate continuous description  
 232 of the defect cores than the per-atom Nye estimation for such defects.

### 233 3.3. Inspection of elastic fields: strain and rotation

234 We will now explore the applicability of the transfer methods in evaluating the elastic strain/rotation fields gen-  
 235 erated by the dislocations and GBs. First, the atomic elastic strain field obtained through the lattice correspondence  
 236 tensor will be qualitatively compared to the continuous elastic fields obtained from FDM simulations, using input  
 237 dislocation densities from the transfer methods. The components of the per-atom strain  $\varepsilon_{ij}$  can be computed from the  
 238 lattice correspondence tensor  $\mathbf{G}$  by

$$\varepsilon_{ij} = ((\delta_{ij} - G_{ij}) + (\delta_{ij} - G_{ji}))/2, \quad (16)$$

239 where  $\delta_{ij}$  is the Kronecker symbol. The figures 4 (a), 4 (b) and 4 (c) represent the distribution of the out-of-plane  
 240 shear component  $\varepsilon_{23}$  of the elastic strain field from a screw dislocations in tungsten. The color scale used in Fig. 4  
 241 represents strain ranging from -7 % to +7 %. It is identical for both atomistic and continuous representations.

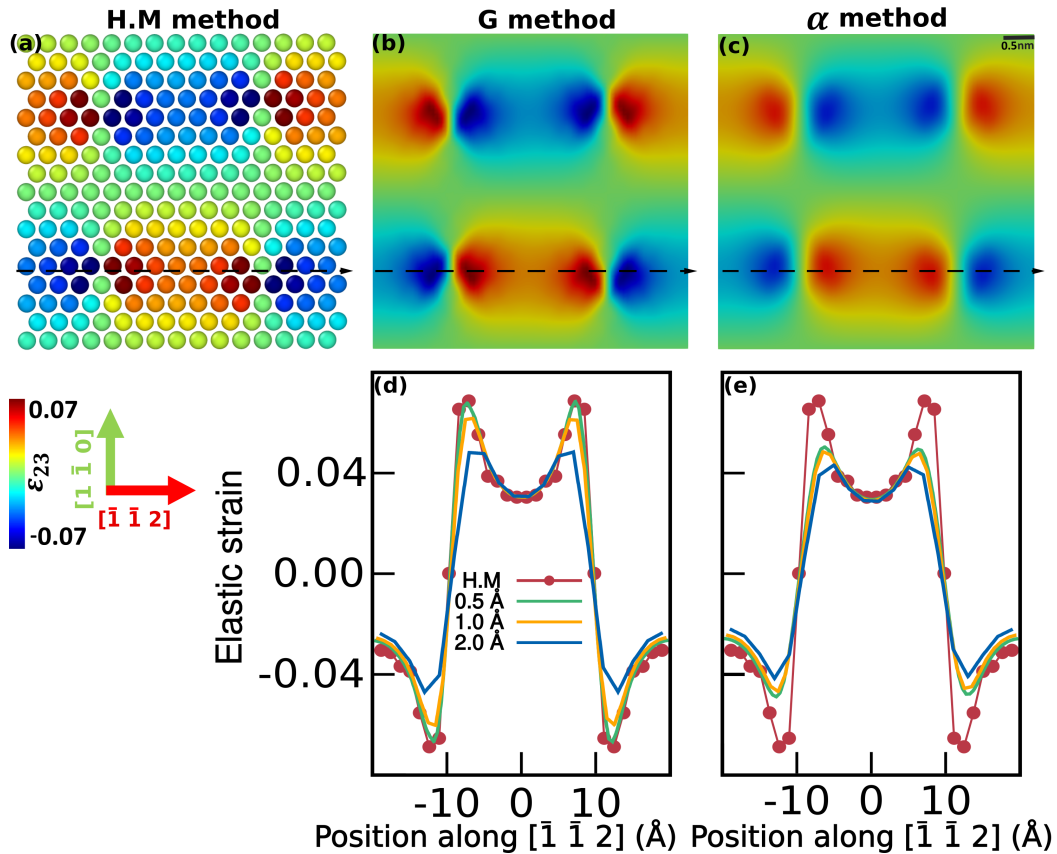


Figure 4: Elastic strain field obtained for screw dislocation quadruple in tungsten with the G and  $\alpha$  transfer methods using a 0.5 Å FFT grid resolution and compared to the HM method atomistic result. (a) Visualization of the per-atom strains  $\varepsilon_{23}$  using Hartley and Mishin method. (b) and (c) Maps displaying the elastic strain fields obtained via the G and  $\alpha$  methods. The dashed lines indicate the directions for plotting profiles. (d) and (e) represent the elastic strain  $\varepsilon_{23}$  profiles along the  $[\bar{1}\ \bar{1}\ 2]$  direction obtained with the G and  $\alpha$  methods.

242

243 In the case of positive screw dislocations, there is positive shear strain on the left side and a negative shear strain  
 244 on the right side of the dislocation core, which qualitatively aligns with the elastic field predicted for a straight  
 245 screw dislocation line in isotropic elasticity. As described earlier, the structural units composing the low-angle grain  
 246 boundary can be seen as an array of edge dislocations. Figures 5 (a), 5 (b) and 5 (c) exhibit the distribution of the  
 247 in-plane shear component  $\epsilon_{12}$  of the elastic strain field of an isolated dislocation in the LAGB. The field acquired by  
 248 both transfer methods closely aligns with the results from atomistic calculations, demonstrating a good agreement  
 249 between both approaches.

250 In the case of the screw dislocations and LAGB however, we observe that the G method much better captures the  
 251 high strain gradients in the immediate core region of defects, while both methods accurately capture the relatively  
 252 smaller strains in regions away from the defect cores.

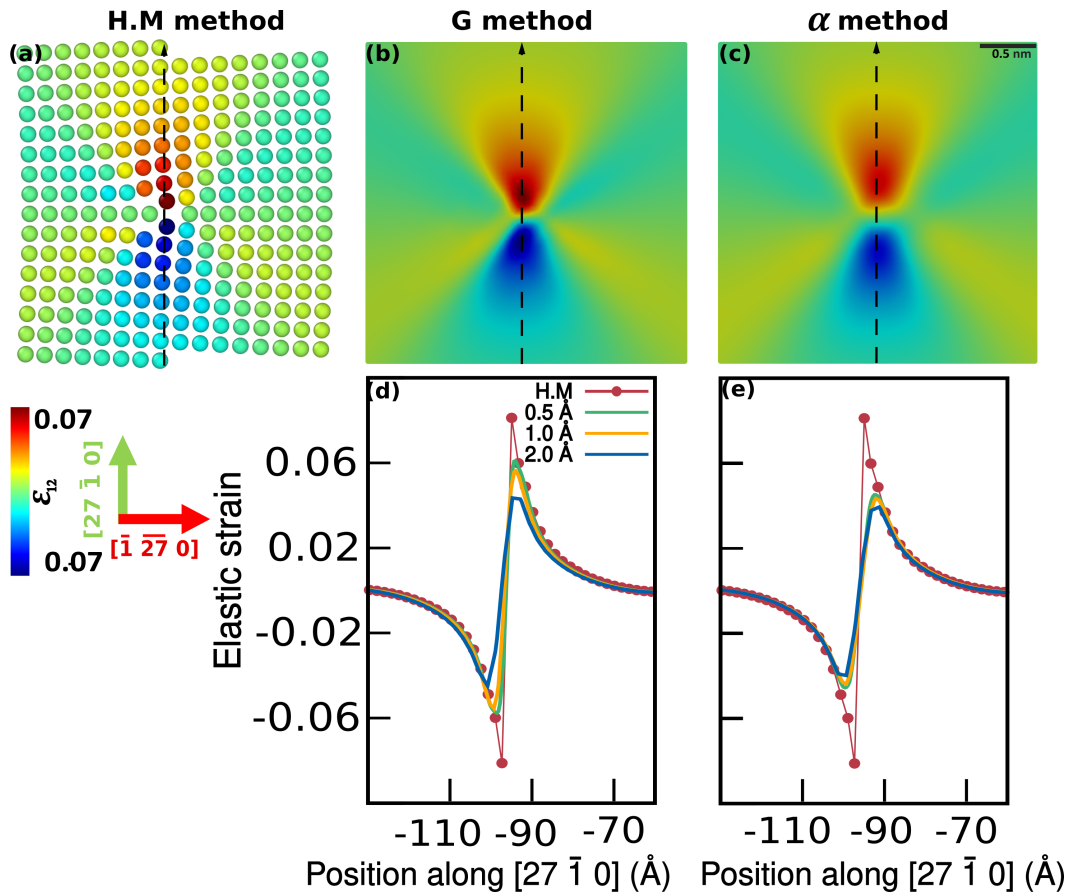


Figure 5: LAGB in copper: Elastic strain field obtained with the G and  $\alpha$  transfer methods using a 0.5 Å FFT grid resolution and compared to the HM method atomistic result. (a) Visualization of the per-atom elastic strain  $\epsilon_{23}$ . (b) and (c) Maps displaying the elastic strain field  $\epsilon_{23}$  obtained via the G and  $\alpha$  methods. The dashed lines indicate the directions for plotting profiles. (d) and (e) represent the elastic strain  $\epsilon_{12}$  profiles along the  $[27 \bar{1} 0]$  direction obtained with the G and  $\alpha$  methods.

253 To quantify these observations, we plot the distribution profiles of the elastic fields  $\epsilon_{23}$  and  $\epsilon_{12}$ , following the  
 254 directions marked with dashed lines on figures 4 and 5 (d). For the screw dislocation cores, figures 4 (d) and 4 (e)  
 255 compare the profiles of the atomic strain field (red solid line with symbols) and the continuous strain fields (solid lines)  
 256 obtained using the G and  $\alpha$  methods respectively, for different FFT grid resolutions. The results show the correct  
 257 reproduction of the significant gradient of strain at dislocations core, with the G method and fine resolutions. The  
 258 ability to capture these core-level strains is degraded at a resolution of 2 Å. The comparison between the atomistic  
 259 and the continuous strain field obtained using the  $\alpha$  method reveals that this approach is not as effective as the G

260 method in capturing the high strain levels near the dislocation core, even when employing the finest resolution. It is  
 261 also noteworthy that the resolution has more effect on the G method than on the  $\alpha$  method, and that both methods  
 262 capture correctly the long-range elastic fields away from the defect cores, whatever the resolution. Similar findings  
 263 apply to the case of the LAGB (Figures 5 (d) and 5 (e)). While the G method reproduces almost perfectly the strain  
 264 fields at the core of screw dislocations obtained from DFT, it is slightly less efficient to reproduce the elastic fields  
 265 observed around the dislocation and structural unit cores within grain boundaries as obtained with semi-empirical  
 266 potentials. Figures 6 (d) and 6 (e) show the profiles of the tilt elastic rotation field, describing the grain boundary  
 267 misorientation angle along the  $[3\ 1\ 0]$  direction, using the G and  $\alpha$  methods, respectively. Both methods effectively  
 268 capture the expected rotation field, the G method providing a slightly better agreement with atomistic results. For the  
 269 finest FFT grid resolution, both approaches converge to a misorientation angle of 0.632 radians, corresponding to the  
 270 characteristic misorientation of the  $\Sigma 5(3\ 1\ 0)[0\ 0\ 1]$  grain boundary considered in this work.

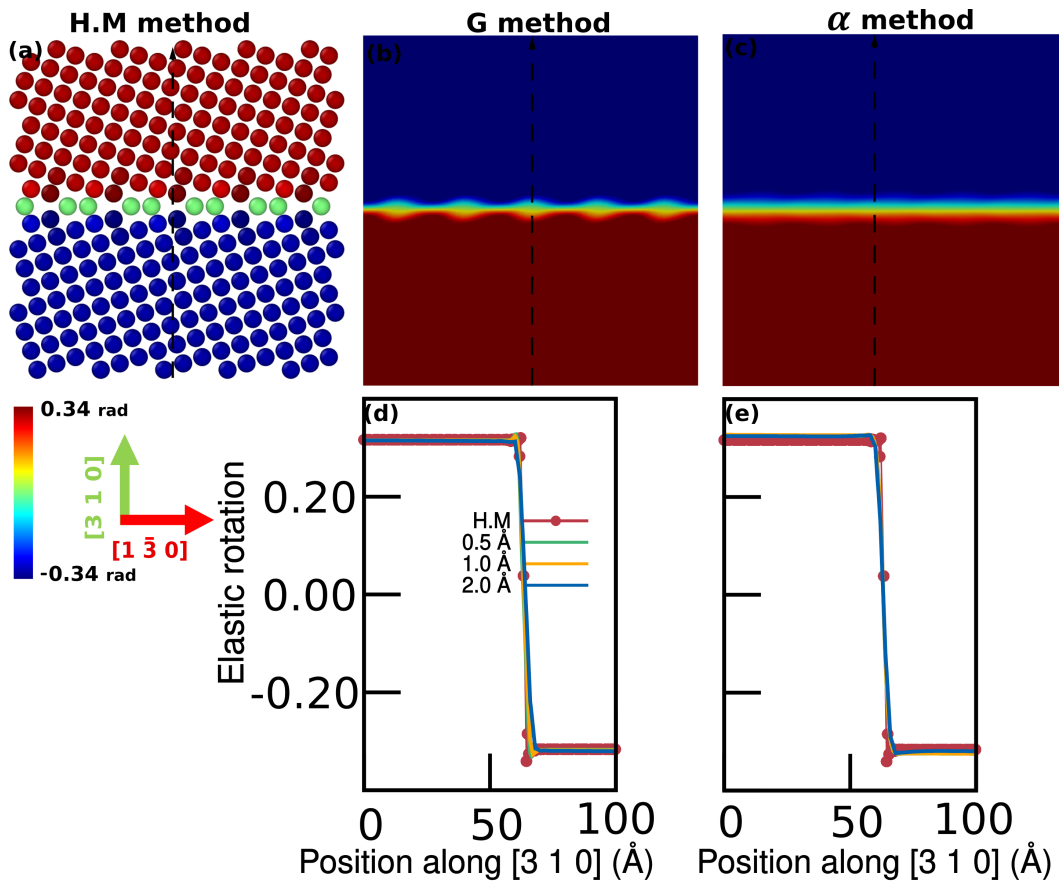


Figure 6: HAGB in copper: Elastic rotation field obtained with the G and  $\alpha$  transfer methods using a 0.5 Å FFT grid resolution and compared to the HM method. (a) Visualization of the per-atom elastic rotation. (b) and (c) Maps displaying the rotation field obtained via the G and  $\alpha$  methods. The dashed lines indicate the directions for plotting profiles. (d) and (e) represent the tilt rotation profiles along the  $[3\ 1\ 0]$  direction obtained with the G and  $\alpha$  methods.

### 271 3.4. Application to dislocation / grain boundary interactions

272 In light of the previous examples, the G method, using a 0.5 Å FFT resolution, demonstrates to be effective  
 273 in capturing the short and long range mechanical fields generated by screw dislocations, low and high angle grain  
 274 boundaries. The next focus involves the application of the G method to investigate the elastic interactions between  
 275  $\Sigma 291(13\ 11\ 1)[1\ 1\ 2]$  symmetric tilt grain boundary and edge extrinsic dislocations in copper. Two molecular static  
 276 simulation scenarios were performed. In the first scenario (Figure 7 (a)), the extrinsic dislocation is aligned with an

277 intrinsic dislocation composing the grain boundary. The two dislocations have opposite sign. In the second scenario  
 278 (Figure 7 (d)), the dislocation is shifted by two  $\{111\}$  planes in such a way that the extrinsic dislocation is aligned  
 279 in between two intrinsic dislocation composing the grain boundary. To bring the systems into equilibrium, the FIRE  
 280 algorithm [42] is used and the configurations were considered optimized when the norm of the global force vector  
 281 is below  $10^{-6}$  eV/Å. Figure S4 (in supplementary materials) describes the details of the systems' configuration using  
 282 the per-atom Nye dislocation density. The Burgers vector norm of dislocations is  $b = 2.56$  Å. This value is calculated  
 283 by integrating the Nye tensor over a rectangular grid in a plane normal to the dislocation line. The G method is  
 284 applied to capture the interactions of the elastic stress fields induced by the inserted edge dislocation and the low  
 285 angle grain boundary, and compared to the virial stress calculated by molecular static simulations. Depending on  
 286 the initial position of the extrinsic dislocation, two distinct interaction scenarios are observed. Figures 7 (b) and (c)  
 287 depict the per-atom virial shear stress and that obtained with the G transfer method, respectively, illustrating the first  
 288 interaction scenario. The extrinsic edge dislocation has annihilated with one intrinsic dislocation composing the GB.  
 289 The grain boundary is indeed described as an array of edge dislocations, where the core of each dislocation undergoes  
 290 slight dissociation into two Shockley partials. This annihilation results in a local increase in the stress field due to a  
 291 reduction in the elastic screening between neighboring intrinsic GB dislocations. In the second scenario, the extrinsic  
 292 dislocation stabilizes near the grain boundary, causing disruption in the dislocation network within the grain boundary  
 293 and slight migration towards the dislocation (Figures 7 (e) and (f)). The short-range elastic interactions between the  
 294 extrinsic dislocation and the GB dislocations is rather well captured by the G method in both scenarios. Note that this  
 295 relaxed configuration is not realistic, as annihilation should likely occur by local climb process. It is not possible here  
 296 as simulations are performed at 0K.

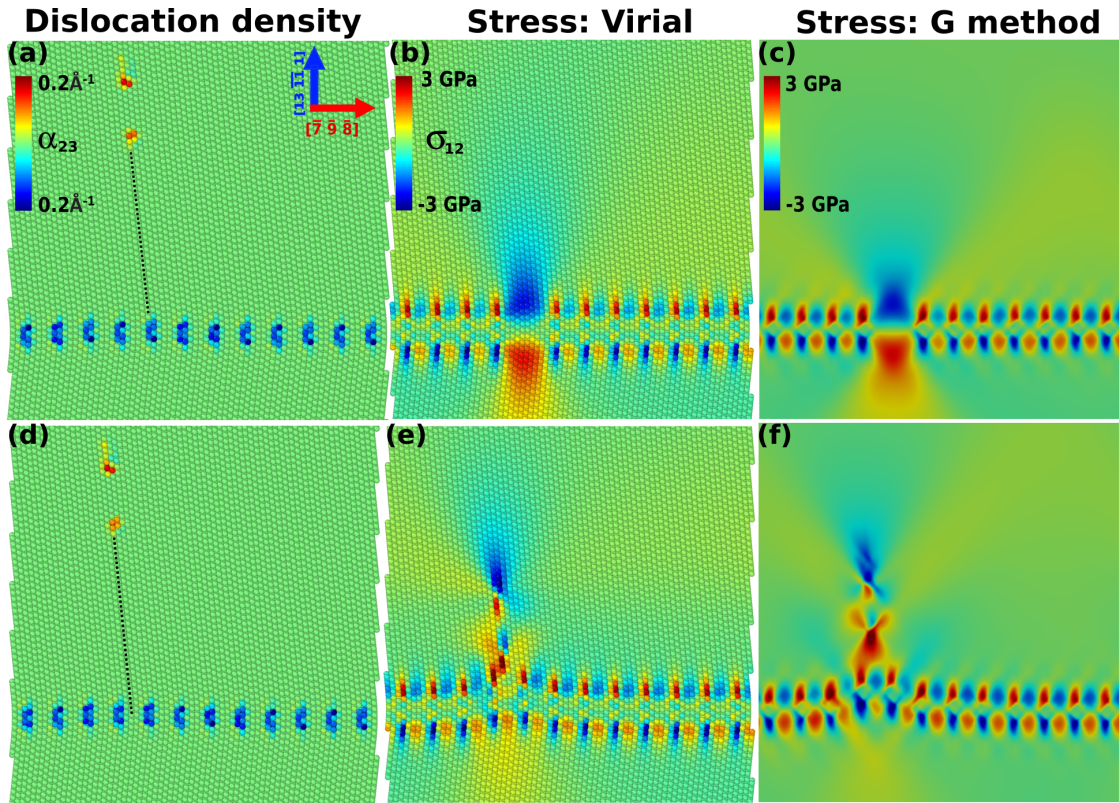


Figure 7: Interaction between an extrinsic edge dislocation and a  $\Sigma 291(13\bar{1}1)1[\bar{1}\bar{1}2]$  low angle STGB in copper, with two scenarios: the edge dislocation will annihilate with one composing the GB (a,b,c); the edge dislocation will stop nearby the GB (d,e,f). Figures (a,d) show the per-atom Nye dislocation density  $\alpha_{23}$  in the initial (unrelaxed) configuration for both scenarios. The dashed black lines indicate the  $\{111\}$  glide plane of the extrinsic edge dislocation. In (b,e) is shown the per-atom virial stress  $\sigma_{12}$  of the final (relaxed) configuration, when the edge dislocation has interacted with the GB, for both scenarios. Figures (c,e) show the same stress fields obtained via application of the G method with a  $0.5\text{\AA}$  FFT grid resolution.

## 297 4. Conclusions and perspectives

298 This paper introduces a new methodology to establish an atomistic to continuum mechanics crossover method,  
299 whereby atomic positions in defected regions are used to derive a continuous Nye dislocation density field that is an  
300 input in a Field Dislocation Mechanics model. This approach is primarily based on the derivation of the per-atom  
301 Nye and lattice correspondence tensors obtained from the Hartley and Mishin method, which we then use as possible  
302 inputs on a FFT grid to derive as best as possible the continuous Nye tensor for FDM simulations. The practical out-  
303 comes of our research underline the effectiveness of the G method, which relies on interpolating the components of  
304 the lattice correspondence tensor as input on the FFT grid. With this method, the FDM model can accurately predict  
305 the Burgers vector of defects, as well as the elastic strain and rotation fields near and away from the defect cores, in  
306 particular in the case of the screw dislocations simulated by DFT. Note also the efficiency of the FDM model, despite  
307 it being formulated within a small strain, linear elastic framework. Another interesting and unexpected result for high  
308 angle grain boundaries with structural units closely packed, is that the latter can be described as localized, equivalent,  
309 edge dislocations. This approach is thus in favor of dislocation based models for GBs and represents a compelling  
310 alternative for modeling high angle grain boundaries without relying on disclination fields [25]. The methodology  
311 was extended to investigate the interactive elastic fields between an extrinsic edge dislocations and a low angle grain  
312 boundary. It highlights how the stress field due to the presence of the dislocation influences the dislocation network  
313 at the grain boundary.

314  
315 A development of our transfer approach could be on polycrystalline materials. While we considered here only  
316 (quasi) 2D configurations, our method is intrinsically 3D and can be extended to study interfacial plasticity, i.e.,  
317 mechanisms related to grain boundary - dislocation interactions. This would allow considering the presence of initial  
318 grain boundary dislocation content and short/long range internal stresses, and the effects on the development of plastic  
319 deformation within grains and at/across GBs. An ongoing development of our approach concerns the assessment of  
320 strain gradient plasticity models based on GND or Nye dislocation density tensor. Such models add supplementary  
321 internal energy functionals based on the Nye tensor to better capture size effects [43] or dislocation transfer mech-  
322 anisms at GBs [7], for instance. By applying our method to excess grain boundary energies measured by atomistic  
323 simulations for various grain boundaries, it is possible to test different energy functionals proposed in the literature  
324 and to quantify the internal characteristic lengths introduced.

### Competing interests

There are no conflicts to declare.

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Supplementary Materials to:  
Atomistic to continuum mechanics description of crystal defects with dislocation  
density fields: application to dislocations and grain boundaries

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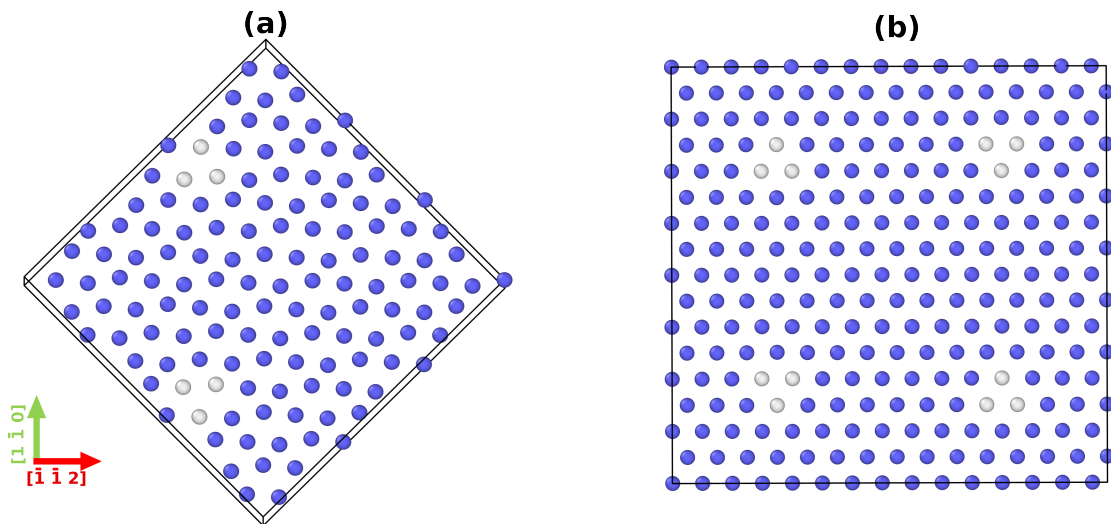


Figure S1: Tungsten simulation cells. Color coding is based on the common neighbor analysis [1]: blue, bcc; white, undefined environment. (a) Visualization of the screw dislocations dipole of opposite Burgers vectors in 135-atom simulation cell generated by DFT. (b) Quadruple of screw dislocations obtained through the periodic boundary conditions applied in all directions to the configuration depicted in (a). Rectangular crop is applied specifically for FFT calculations.

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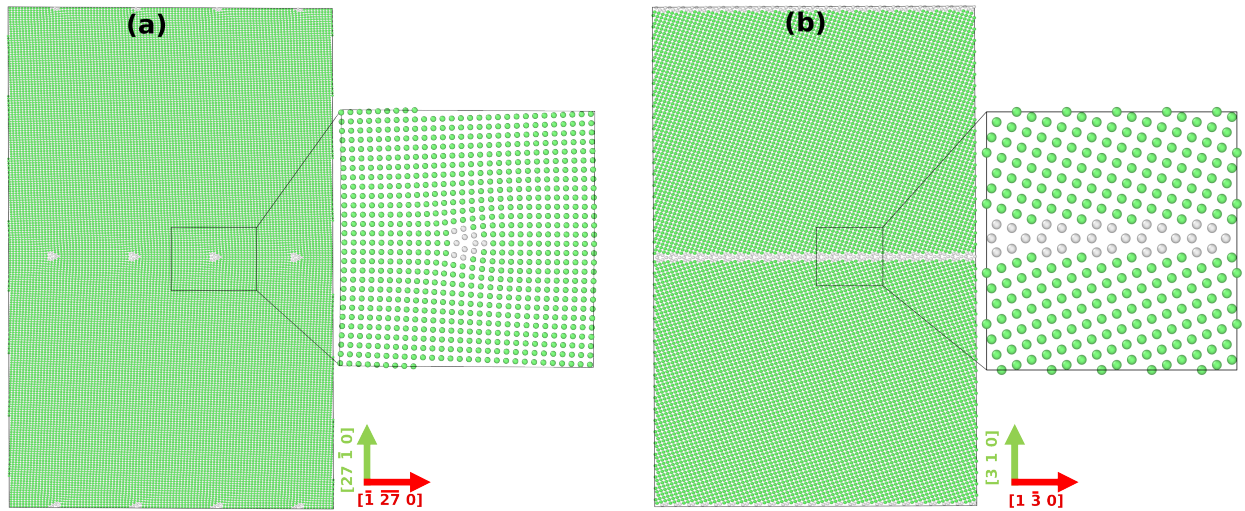


Figure S2: Snapshots of the atomistic simulation cells used for the grain boundaries calculations. Atoms are colored following the local structural type: green, FCC structure; white, undefined structure. a) Low angle grain boundary in copper. b) High angle grain boundary in copper

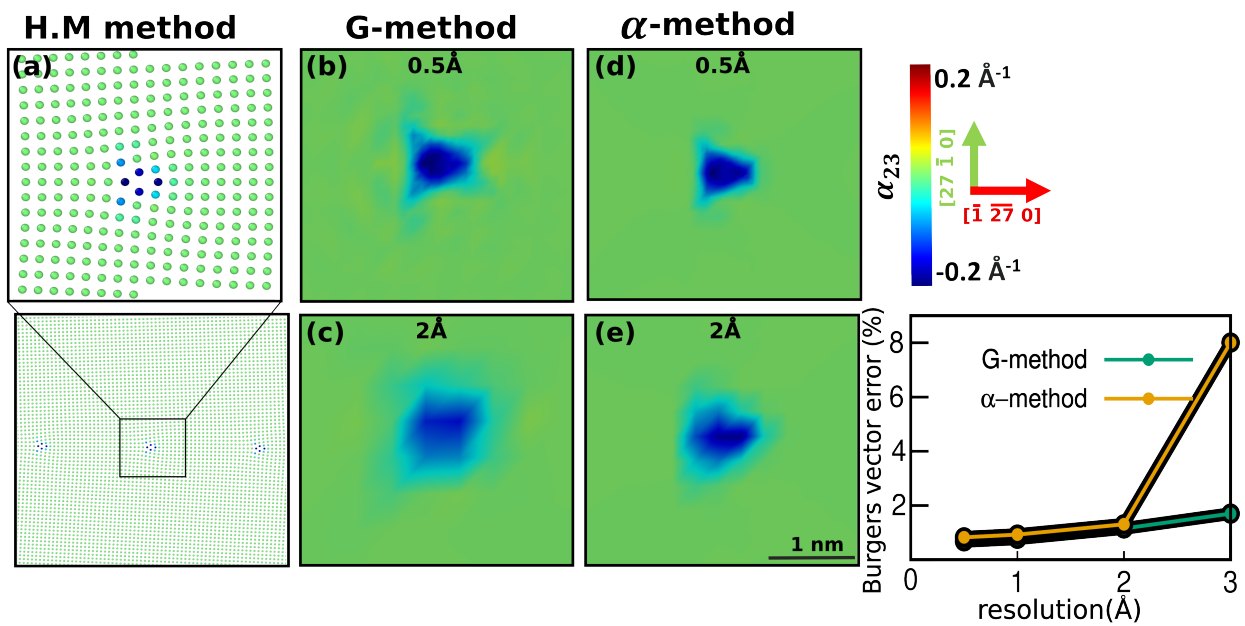


Figure S3: Edge dislocations within low angle grain boundary. Effect of FFT grid resolution on Nye dislocation density distributions and Burgers Vector norm error using G and  $\alpha$  methods. (a) Visualization of the per-atom component  $\alpha_{23}$  of the Nye tensor as obtained from the Hartley-Mishin method. (b) and (c): maps illustrating the edge dislocation density distribution obtained using the G-method with FFT Grid resolutions of 0.5 Å and 2 Å, respectively. (d) and (e) depict edge dislocation density distributions using the  $\alpha$  method with 0.5 Å and 2 Å FFT grid resolutions. (f) The variation of the Burgers vector norm error as a function of the grid resolution using the G-method (Green line) and  $\alpha$  method (Yellow line).

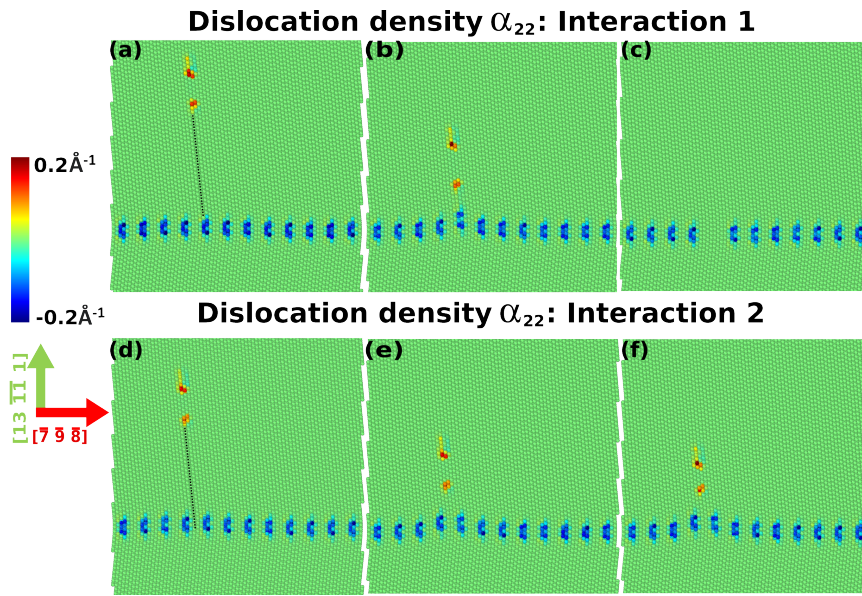


Figure S4: Interaction between extrinsic edge dislocation and  $\Sigma 291(13 \bar{1} 1)[\bar{1} \bar{1} 2]$  STGB in copper: Visualization of the per-atom  $\alpha_{23}$  Nye density during molecular static minimization. The GB is created initially by rotating two crystal lattices oriented along the x[1  $\bar{1}$  0], y[1 1 1], and z[ $\bar{1}$   $\bar{1}$  2] directions around the z-axis by angles of  $\theta/2 = 5.83^\circ$  and  $-\theta/2 = 5.83^\circ$ , respectively. An energy minimization is performed, using the FIRE algorithm [2], to obtain the grain boundary relaxed structure. The edge dislocation line is aligned parallel to the z-axis. The Burgers vector is set at  $b = 2.55 \text{ \AA}$  within a (1 1 1) plane. (a, b, d, e) depicting the dislocation density distribution in unstable configurations, observed when the norm of the global force vector  $f_c$  exceeds  $10^{-6} \text{ eV/\AA}$ . (c, f) illustrates the relaxed configuration with a global force vector norm below  $f_c$ .

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