Representation of mechanical loads in molecular dynamics simulations

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We describe a constant-traction molecular dynamics method to perform simulations of a generic atomistic system under an applied external load. The main objective is to ensure consistency between the atomistic model and the macroscopic continuum-mechanics description. Examples of simulations for different kinds of extended defects under an external load, such as a grain boundary, an elliptical microcrack, and a screw dislocation in a fcc crystal are presented, and compared with the results of the corresponding continuum mechanics description.

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I. INTRODUCTION

The study of the mechanical response of materials under an external load has recently grown to a subject of fundamental research, mainly thanks to the possibility of performing fully atomic-scale simulations of very large systems containing extended defects, such as microcracks, dislocations, and grain boundaries.[1,2] The key issue in the atomic-level description of a system under an externally applied mechanical load, i.e., under a given state of macroscopic stress, is to ensure that the border conditions of the simulation cell properly represent the type and magnitude of the external load. As we shall see, this problem is closely connected with the suppression of system-size effects such that the far-away stress and strain fields surrounding the typically very small region of interest, e.g., enclosing one or more dislocations or microcracks, converge to the proper linear-elasticity limit for any given state of loading.

Since any practically realizable atomistic system is of very small size, real-world extended systems are usually represented in molecular dynamics (MD) simulations by means of periodic border conditions (BC) applied to the box enclosing the atomistic system.[3] Periodic BC may, however, induce spurious effects due to the fact that the atoms in the box interact with each other and with all their periodic replicas. For long-range fields, such as the elastic field of a dislocation, which decays as r^{-1}, or that of a microcrack, which decays as $r^{-1/2}$, this approach leads to the so-called problem of the image forces, namely the defect fictitiously interacting with itself infinite times, leading to a divergence in the total energy. In the recent literature this problem has been usually circumvented by studying particular clusters of defects, e.g., a dislocation dipole or quadrupole with properly arranged Burgers vectors,[2] such that the long-range stress fields approximately cancel out. Clearly, one should aim at a more general framework in which, moreover, consistency with macroscopic continuum mechanics is ensured.

The problem of simulating an atomistic system in a well-defined state of *homogeneous* stress was boldly solved by the so-called Parrinello-Rahman (PR) formulation of constant-stress MD.[4] The PR method is a special type of periodic BC in which the total stress (a Cartesian tensor) acts as a nine-component constraint determining the dynamic evolution of the size and shape of the (periodic) simulation box. However, in a discrete system the total stress can be obtained only as a sum over some ''atomistic'' stress tensor (see below), which is derived by breaking down the total stress into the contributions of equivalent atoms.[5] By contrast, defects such as dislocations or microcracks tend to concentrate the stress field, thus making the system elastically inhomogenous. Consequently, as clearly stated already in the original paper,[4] the PR method is suitable only for a homogenous system.

Alternate forms of BC's have thus been devised to deal with extended defects in atomistic systems under a mechanical load: (a) *constant-displacement* or fixed-boundary BC,[6–8] in which the border atoms are held in the strained configuration or, equivalently, periodicity is preserved across the border for the whole duration of the simulation; (b) *constant-traction* BC,[9–11] in which periodicity is removed all around the borders and the equivalent forces necessary to preserve the state of deformation are computed and applied to the border atoms during the simulation. The above classes of BC correspond, respectively, to the displacement-boundary value (or Dirichlet) and to the stress-boundary value (or Neumann) formulations of continuum mechanics problems, in which either displacements or stresses are prescribed along the system borders.

In this work we describe an atomistic simulation scheme to apply a general external load to a finite-size, nonperiodic atomistic system while reproducing the loading conditions of an infinite continuum. Such a scheme, previously developed at zero temperature[10,11] and here generalized to finite temperatures, is based on the definition of an atomic-scale *surface traction* perfectly equivalent to its continuum-mechanics analog. The surface traction is applied as a constant external force to the free (i.e., nonperiodic) borders of the atomistic system, hence the denomination of ''constant-traction BC.'' As an additional benefit, we will show that the constant-traction BC under zero external load represents a practical way to embed an intrinsically nonperiodic atomistic system, e.g., a dislocation or a triple junction,[12] in a virtually infinite medium.

II. CONSTANT-TRACTION METHOD

The most important quantity to compare the atomic-level and continuum mechanics description of a system under ex-

ternal load is the stress tensor. In the context of atomistic simulations it is customary to calculate the so-called virial stress tensor $\Sigma_{\alpha\beta}$:[3–5]

$$\Omega\Sigma_{\alpha\beta}=\sum_i \frac{p_i^\alpha p_i^\beta}{m_i}-\sum_{i<j}\frac{1}{r_{ij}}\frac{\partial V}{\partial r_{ij}}r_{ij}^\alpha r_{ij}^\beta, \tag{1}$$

where $\alpha,\beta=x,y,z$ denote Cartesian components and the sums extend over all the atoms in a simulation box of total volume Ω; m_i and p_i are the mass and linear momentum of atom i, respectively, and r_{ij} is the relative distance between atoms i and j interacting via a pair potential $V=V(r_{ij})$; we note that both Eq. (1) and the following expressions are easily generalized to more complex interatomic potentials. Moreover, it is worth noting that the virial expression provides the product quantity $\Omega\Sigma_{\alpha\beta}$ and not the stress tensor alone.

The most obvious prescription to calculate the individual terms of the sum in Eq. (1) for a crystal lattice of N atoms enclosed in a periodic box, is to subdivide the total system volume into equal atomic volumes, $\omega=\Omega/N$, thus defining an atomic-level stress tensor $\sigma_{\alpha\beta}^i$:

$$\sigma_{\alpha\beta}^i=\frac{1}{\omega}\left(\frac{p_i^\alpha p_i^\beta}{m_i}-\sum_j \frac{1}{r_{ij}}\frac{\partial V}{\partial r_{ij}}r_{ij}^\alpha r_{ij}^\beta\right) \tag{2}$$

such that

$$\Sigma_{\alpha\beta}=\frac{1}{\Omega}\sum_i \omega\sigma_{\alpha\beta}^i. \tag{3}$$

Strictly speaking, the above expression is well defined only for a system of perfectly equivalent atoms, i.e., a homogeneously stressed system. However, it has been frequently used also for nonhomogeneous systems, e.g., to calculate the stress around a dislocation. Apparently, this was attempted by Basinski *et al.*[13] and subsequently by many others, by replacing ω (or better, ω_i) with, e.g., the volume of the Wigner-Seitz or Voronoi cell centered at each atom.

The inadequacy of Eq. (2) for systems containing either pointlike or extended defects was clearly exposed by Lutsko[14] and Cheung and Yip,[15] both which suggested alternative prescriptions for defining an atomic-level stress tensor to account for nonequivalent atoms. More recently, another definition of atomic-level stress was introduced[16] which appears to satisfy conservation of linear momentum. In fact, the commonly used definition of Eq. (2) is known to give unphysical results, e.g., when approaching a free surface or a grain boundary. It must be noted that the PR method requires us to calculate the total stress in the simulation box, i.e., for a system including extended defects it would include also the contribution of regions in which the expression (2) is ill defined.

The constant-traction BC which we are now going to describe does not rely upon the explicit evaluation of the atomic-level stress, and this is quite an advantage in view of the above discussion. We consider a static external load, ideally applied at infinite distance from the region of interest, represented by a homogeneous deformation tensor $\epsilon_{\alpha\beta}$ applied to the atomistic system as a whole. The corresponding stress tensor is easily obtained as $\sigma_{\alpha\beta}=\Sigma_{\gamma\delta}C_{\alpha\beta\gamma\delta}\epsilon_{\gamma\delta}$ which is a generalized Hooke's law with the point-group symmetry of the crystal lattice, the matrix of elastic constants $C_{\alpha\beta\gamma\delta}$ playing the role of a four-index tensorial spring constant.[5]

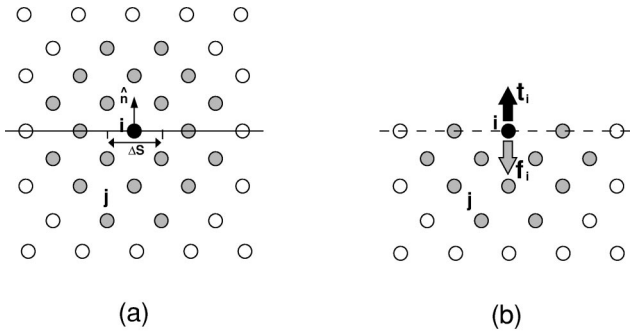

FIG. 1. Schematic of the forces acting on a border atom. (a) Periodic border: all the neighbors within the cutoff radius (shaded atoms) contribute to the force on atom i, $\mathbf{f}_i=0$. (b) Free border: the presence of only part of the neighbors, j, results in a nonzero bulk force $\mathbf{f}_i$ which gives the surface traction $\mathbf{t}_i=-\mathbf{f}_i$.

The Cartesian component of the force on each atom i induced by a pair potential $V(r_{ij})$ is

$$f_i^\alpha=\sum_j\left(-\frac{1}{r_{ij}}\frac{\partial V}{\partial r_{ij}}\right)r_{ij}^\alpha. \tag{4}$$

At mechanical equilibrium each component of the net force on each atom is zero. Now, the analogy between the constant-traction BC and the removal of periodicity across a border can be understood with the help of Fig. 1. Figure 1(a) represents the usual periodic (or constant-displacement) BC: the horizontal line defines the limit between the portion of the system explicitly simulated and its periodic replica. When an initial deformation $\epsilon_{\alpha\beta}$ is imposed on such a periodic system, equal and opposite forces are induced on each atom i from its displaced neighbors j, ending up with a zero net force and thus with no additional displacement with respect to the imposed deformation. It is worth underscoring that, although the atoms experience a state of nonzero stress, they keep the deformed configuration because $f_i^\alpha=0$ for every atom. Figure 1(b), in turn, represents the constant-traction BC: after imposing the homogeneous deformation $\epsilon_{\alpha\beta}$ to the system, periodicity in the direction normal to the border is suppressed, i.e., atoms in the region above the dashed line (indicating a free border) are removed. The effect of these ''missing'' atoms can be mimicked by a suitable external force $\mathbf{t}_i$ to be applied to the border atoms for the whole duration of the simulation. This is nothing but the Cauchy-Euler principle of continuum mechanics,[17] stating that the action of the material occupying the part exterior to a closed surface onto the material occupying the interior part is represented by a vector field $\mathbf{t}_i$, called the *surface traction*.

By substituting Eq. (4) in the virial definition, Eq. (2), for the atomic-level stress and noting that at zero temperature the kinetic contribution is zero, it is easily shown that the *opposite* of the net resulting force $-f_i^\alpha$ is equivalent to a

surface force parallel to the surface normal n^β tending to preserve the state of deformation:

$$t_i^\alpha = \int_{\Delta S} (\sigma_{\alpha\beta}^i \cdot n^\beta) dS = -f_i^\alpha . \tag{5}$$

We note that this procedure for obtaining a surface traction from the opposite of a bulk force is analogous to the image-field method, widely used in continuum mechanics to obtain a special solution for singular boundary-value problems.[17] Such a procedure has been used, e.g., in the finite-element solution for the problem of finding the equilibrium distribution of a collection of discrete dislocations in a linear elastic medium.[18] Moreover, we underscore that Eq. (5) does not depend on the particular definition of atomic-level stress adopted, since one can directly obtain the value of **t** from the bulk force **f** without having to explicitly calculate $\sigma_{\alpha\beta}$.

In this respect, the central observation is that the total stress is generally linked to the tensorial first derivative with respect to the deformation of the internal energy, $U = \Sigma_i U_i$, by the thermodynamic relation[19]

$$\Sigma_{\alpha\beta} = \frac{1}{\Omega} \sum_i \frac{\partial U_i}{\partial \epsilon_{\alpha\beta}} = -\frac{1}{\Omega} \sum_i f_i^\alpha r_i^\beta \tag{6}$$

independently on the particular atomistic definition chosen for $\sigma_{\alpha\beta}$.

At finite temperatures the surface traction must be obtained by a statistical ensemble average. Indeed, mechanical equilibrium at $T>0$ is imposed by requiring that the *average* force on each atom is zero:

$$\langle \mathbf{f}_i \rangle = \frac{1}{Z} \sum_i \int d\Omega e^{-U/k_B T} (-\nabla_i V) = 0 \tag{7}$$

with $Z = \int d\Omega \exp(-U/k_B T)$.

For the atoms at the nonperiodic border of Fig. 1(b) the mechanical equilibrium is written

$$\frac{1}{Z} \left(\sum_{i'} \int d\Omega e^{-U/k_B T} (-\nabla_i V) + \int d\Omega e^{-U/k_B T} \mathbf{t} \right) = 0, \tag{8}$$

where the prime indicates that the sum runs only on the remaining neighbors after removal of the periodicity.

We note that the modulus and direction of the surface traction are uncorrelated in the thermal motion of border atoms, i.e., the three Cartesian components of **t** fluctuate independently. So we can write $\mathbf{t} = t\hat{\mathbf{n}}$, with $\hat{\mathbf{n}}$ being the unit vector defined in Fig. 1, to obtain

$$\langle \mathbf{f}_i \rangle + \langle t\hat{\mathbf{n}} \rangle = \langle \mathbf{f}_i \rangle + \langle t \rangle \langle \hat{\mathbf{n}} \rangle = 0 \tag{9}$$

from which the surface traction is formally defined as

$$\langle t \rangle \langle \hat{\mathbf{n}} \rangle = -\langle \mathbf{f}_i \rangle . \tag{10}$$

The above expression states that the average surface traction is equal in modulus to the average missing force (since $\hat{\mathbf{n}}$ is a unit vector) and is directed as the average value of the surface normal. Furthermore, Eq. (10) also suggests an operational definition of the instantaneous surface, to be identified with the plane perpendicular to the instantaneous missing force.

In practice, the constant-traction MD method works in two separate steps: (i) the modulus of the average missing force is obtained in a separate bulk calculation at finite temperature during which the atomic force across any dividing plane $\{hkl\}$ can be calculated; (ii) the surface traction is applied during the subsequent simulation to each border atom with a constant modulus corresponding to the given value of T and directed as the opposite of the instantaneous resulting force $\mathbf{f}_i$.

III. COMPUTATIONAL TESTS OF THE METHOD

As a first test we run a microcanonical MD simulation of 8000 Si atoms described by the Stillinger-Weber interatomic potential.[20] An isotropic, triaxial strain $\epsilon_{\alpha\beta} = \epsilon_0 \delta_{\alpha\beta}$ at the initial temperature $T = 500$ K was imposed to the atomic system, initially arranged with the diamond fcc symmetry in a cube of side $10a_0 = 5.43$ nm with either periodic or constant-traction BC in the three directions. We compared several quantities, e.g., the instantaneous temperature, energy and root-mean-square displacement averaged over the atoms in the inner portion of the simulation box. We found virtually no difference between the simulation with either periodic or constant-traction borders for such a homogeneous, defect free system, i.e., the constant-traction BC provides an effective embedding of the atomistic system in an infinitely extended medium. Moreover, such a simulation is a proof that the constant-traction BC indeed gives an unbiased sampling of the microcanonical ensemble for the atoms far from the boundary.

As a second test we performed a MD simulation of a $\{113\}$ symmetric tilt grain boundary in fcc Cu. We used a simple Lennard-Jones (LJ) pair potential, with parameters $\epsilon = 0.167$ eV and $\sigma = 2.405$ Å, resulting in an equilibrium lattice parameter $a_0 = 3.615$ Å. The grain boundary is placed in the x-y plane at $z = 0$ in a three-dimensional (3D) periodic simulation box. The simulation was run with both the constant-traction BC and the PR method under a uniaxial external load described by the stress tensor $\Sigma_{\alpha\beta} = \Sigma_0 \delta_{\alpha z} \delta_{\beta z}$ and $\Sigma_0 = 0.1E$, with $E = 0.167$ Mbar the theoretical Youngs modulus of our LJ potential. In the constant-traction MD run the periodicity along z was removed. The initial minimum-energy configuration of the grain boundary was obtained by simultaneously optimizing the individual atomic positions and the relative translation between the two half crystals at $T = 0$;[21] then, the deformation was imposed, the system was annealed at $T = 100$ K for about 10 ps and subsequently quenched down to zero temperature.

In Fig. 2 we show the σ_{zz} component of the stress calculated from Eq. (2), averaged over slices of width $\Delta z = 0.25a_0$. The central result is that the constant-traction BC is able to preserve (by construction) the bulk state of stress at sufficiently large distances from the grain boundary, independently on the particular definition adopted to calculate the

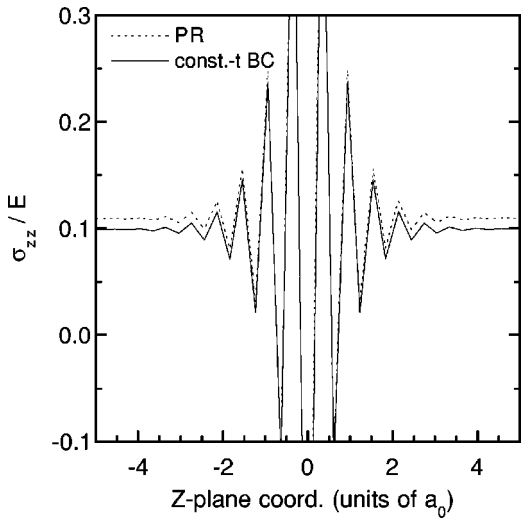

FIG. 2. Plot of the plane-averaged σ_{zz} component of the stress field (in units of the Youngs modulus E) across a $\{113\}$ symmetric-tilt grain boundary in a Lennard-Jones fcc crystal. The dashed line represents the result of a Parrinello-Rahman simulation, the continuous line is the result of a constant-traction simulation, both at $T=0$ K.

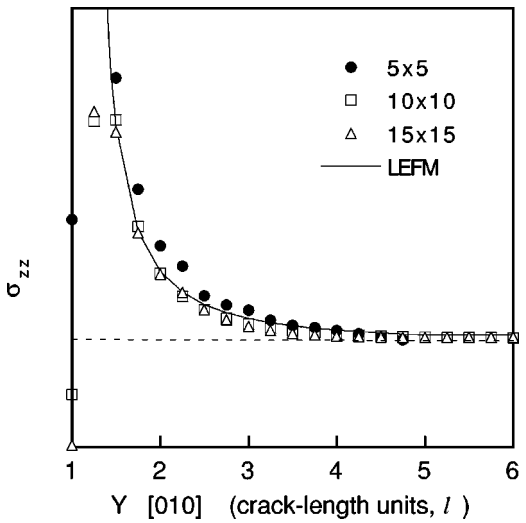

FIG. 3. Plot of the σ_{zz} component of the stress field around an elliptical $\{001\}\langle 010\rangle$ microcrack in a Lennard-Jones fcc crystal. The stress is plotted along the y [010] direction, starting from the crack tip. Symbols represent the results of constant-traction simulations at $T=100$ K followed by quenching at $T=0$ K for various system sizes. The full line is the result of the continuum, anisotropic linear-elasticity solution. The dashed line is the asymptotic value of external stress.

atomic-level stress in the core region. By contrast, the PR solution in the far field contains a small, but nonzero level of excess stress which results from the average of the bulk and grain-boundary regions. For both cases it can be seen that the definition (2) gives rise to wild changes of sign in the stress as the boundary plane, $z=0$, is approached, just as it is found to occur at free surfaces.[15] Now, for an interface or a surface the perpendicular stress should vanish at mechanical equilibrium. However, any atomistic definition of stress incorporates some averaging volume, and it is this volume-averaged quantity that must vanish, not necessarily its pointwise value. Indeed, in this framework there is no way of establishing whether such an oscillatory behavior is a physically meaningful result or it is a mere numerical artifact.

In principle, the discrepancy of the far-field stress in the PR simulation can be fixed by increasing the simulated system size up to the point where the far-field stress is well converged to the value of the applied external load. It could thus be objected that the constant-traction BC is not much different, since it needs as well to be verified against the system size. However, in the case of the constant-traction BC we are taking as a measure of convergence the pointwise value of the stress field in the (linear-elastic) region far away from the defect, and not its integral over the entire system as it is required in the PR method: this removes any difficulty connected with the particular definition and explicit evaluation of the atomic-level stress tensor.

In a previous work[10,11] we applied the constant-traction BC at $T=0$ to study the stress and strain fields around a finite-size microcrack in fcc Cu with the same LJ potential. In that study we demonstrated that the correct stress-strain solution from anisotropic linear-elastic continuum theory of fracture mechanics (or LEFM, Ref. 22) is recovered in the atomistic model already at system sizes of about 10–20 l, with l the length of the microcrack. The microcrack has the $\{001\}\langle 010\rangle$ orientation, i.e., the x-y plane coincides with the crack plane and the crack tip moves along the y direction. The external uniaxial load perpendicular to the crack plane, i.e., along the z [001] direction, is also in this case $\Sigma_0 = 0.1E$. Figure 3 shows the σ_{zz} component of the stress along the y [010] direction, as obtained from a MD simulation at $T=100$ K of the microcrack embedded in systems of increasing size. Each atomistic system is periodic in x-y while a constant-traction BC is applied in z. In the same figure we report also the LEFM solution for the problem of an elliptical crack in a 2D anisotropic plate[22] with the input values of Youngs modulus and surface energy corresponding to our LJ potential. As amply discussed already in Refs. 10 and 11, the constant-traction BC nicely matches the LEFM solution provided the system size is large enough. The only exception is the immediate vicinity of the crack tip, where the discrete nature of the crystal lattice dominates and the stress tensor, Eq. (2), becomes ill defined.

Similar results can be obtained for any other extended defect, e.g., dislocations. As an example, in Fig. 4 we plot the σ_{zz} component of the stress field around a screw dislocation with Burgers vector b parallel to the z axis (corresponding to the fcc [001] direction); the system is again fcc Cu with the same LJ potential above. The dislocation is created by initially applying the displacement field from the anisotropic linear-elasticity solution[23] to each atom, including the core region. The system is subsequently relaxed by a conjugate gradient procedure at $T=0$ and using the constant-traction BC in the x-y plane, while the z direction is kept periodic. It is seen that the asymptotic $1/r$ decay of the Volterra solution for the stress field is correctly recovered already at system sizes of the order of $40b$. Remarkably, the constant-traction BC allows us to represent an isolated dis-

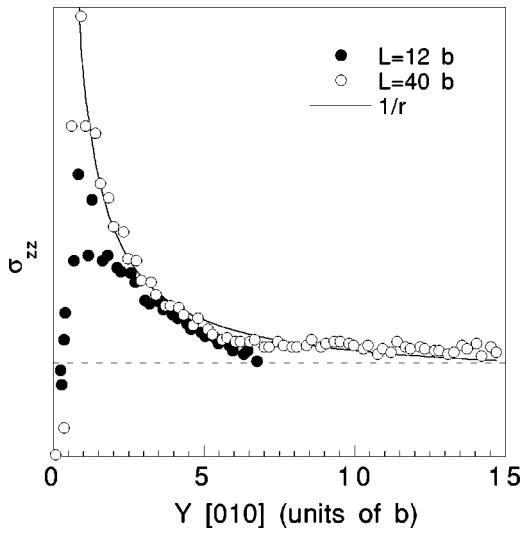

FIG. 4. Plot of the σ_{zz} component of the stress field around a screw dislocation in a Lennard-Jones fcc crystal, with the Burgers vector parallel to the z [001] direction. The stress is plotted along the y [010] direction, starting from the dislocation core. Symbols represent the results of constant-traction simulations at $T=100$ K followed by quenching at $T=0$ K for various system sizes. The full line is the result of the continuum, anisotropic linear-elasticity solution. The dashed line is the asymptotic value of external stress.

location in an infinite bulk, thus removing the problems connected with the image forces implicit in the use of standard periodic BC.[2]

Whenever the initial deformation $\epsilon_{\alpha\beta}$ (or, equivalently, the external stress) is zero the constant-traction BC is able to provide the correct embedding in an infinite, unperturbed medium. In this respect, the constant-traction MD method is also a practical way around the problem of representing nonperiodic defects within a finite-size simulation box. We already used the constant-traction BC at zero load to study the structure and elastic behavior of triple junctions in Si,[12] i.e., the linear defect formed by the joining of three grains with different relative misorientation. This is a typical example of defect for which it is geometrically impossible to build a periodic simulation box except for a few, very special orientations of the grains. Figure 5 shows the minimum-energy configuration of the multiple twin junction formed by two nonequivalent {113} twin boundaries and one {112} symmetric tilt boundary, the $(\bar{1}10)$ x direction (perpendicular to the page) being the common polar axis. The latter direction was periodic while constant-traction BC's were applied in the y-z plane. The configuration was obtained after annealing at $T=500$ K for 40 ps followed by quenching at $T=0$, again using the Stillinger-Weber potential for Si. Such MD simulations performed both at $T=0$ and finite temperatures demonstrate the applicability and usefulness of the constant-traction BC also in such a peculiar system.

IV. CONCLUSIONS

We presented a method to perform molecular dynamics simulations of a fully atomistic system under an externally

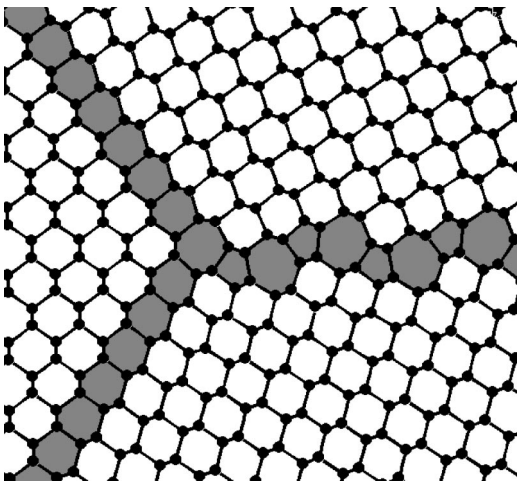

FIG. 5. Minimum-energy atomic structure of a multiple-twin junction in Si obtained after a constant-traction MD simulation; only a central portion of the nonperiodic 9052-atom system projected in the y-z plane is represented. Shaded rings indicate the grain boundaries: the two nonequivalent {113} twins (left) and the {112} symmetric tilt boundary (right), obtained by rotation about the common (110) polar axis (perpendicular to the figure).

applied load. The so-called ''constant traction'' method is based on the evaluation of border tractions (additive forces) to be applied to the atomistic system during the whole simulation, in analogy with the Cauchy-Euler principle of continuum mechanics. We elaborated over our previous work[11] in order to provide an extension of the constant-traction method also to finite-temperature simulations. Several tests of the method on atomistic systems containing different kinds of extended defects, such as a dislocation, a microcrack, and a grain boundary, demonstrated the capability of the method to describe a system under a mechanical load with the proper decay of the far-field stress (i.e., away from the region surrounding the defect) in perfect agreement with the requirements of linear elasticity.

A first relevant feature of the constant traction method is that its application does not require the explicit definition and evaluation of some atomic-level stress tensor. This is definitely an advantage over existing methods, e.g., the Parrinello-Rahman (PR), for nonhomogeneous systems such as a supercell enclosing extended defects. In fact, it has been repeatedly shown that all pointwise definitions of atomic-level stress fail in the immediate neighborhood of defects.[14–16] By comparing simulations with the constant-traction and the PR methods, we clearly demonstrated that the stress field calculated with a PR simulation contains a spurious contribution originating from the highly nonlinear core region of the defect, where the stress tensor is ill defined. Such a problem is absent in the constant-traction method by construction, since it relies only on the evaluation of forces.

A second important feature is that the constant-traction border condition provides the correct embedding in an infinite medium in absence of periodicity. This is of great importance for the simulation of nonperiodic defects with a finite-size simulation box, both under a mechanical loading and load free. We demonstrated the applicability of the

method by simulating nonperiodic defects such as an isolated screw dislocation and an isolated triple junction among three grain boundaries.

Under this latter respect, the constant-traction method should compare well also against the so-called ''hybrid'' approaches, which couple atomistic molecular dynamics with continuum methods such as finite elements.[24,25] Such a coupling can be done by introducing an intermediate region within which atoms and finite elements are linked together by means of a subtle boundary condition.[24] Differently from such approaches, in our method there is no need to introduce an explicit connection between the fully atomistic region and a continuum region, instead the condition of continuity being ensured by the vanishing of the total forces at the free borders. A more advanced option in hybrid methods is the ''quasicontinuum'' approach,[25] in which the atomistic and continuum regions are smoothly linked by means of an interpolation scheme based on the atomistic definition of total energy. Such an approach, indeed, overcomes the problem of introducing an arbitrary link between a discretized and a continuum region. However, it has major difficulties in being extended from $T=0$ to finite temperatures for which, as we demonstrated, the constant-traction method instead performs equally well.

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