Quasicontinuum Models of Interfacial Structure and Deformation

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Microscopic models of the interaction between grain boundaries (GBs) and both dislocations and cracks are of importance in understanding the role of microstructure in altering the mechanical properties of a material. A recently developed mixed atomistic and continuum method is extended to examine the interaction between GBs, dislocations and cracks. These calculations elucidate plausible microscopic mechanisms for these defect interactions and allow for the quantitative evaluation of critical parameters such as the stress to nucleate a dislocation at a step on a GB and the force needed to induce GB migration.

With the continuing development of more accurate, less expensive models for atomistic interactions and expansion of computational resources, there is growing interest in the modeling of materials from fundamental principles rather than phenomenological approaches. An outstanding problem in this regard is the role of microstructure in determining material properties. The influence of microstructure (e.g. grain size and shape) on the mechanical properties of materials is clearly revealed, for example, in the yield strength and the fracture toughness [1]. A first step in the microscopic determination of the role of microstructure in governing such properties is the elucidation of plausible mechanisms whereby dislocations and cracks, the primary agents of permanent deformation, interact with the boundaries that make up that microstructure. One of the key challenges posed by such calculations is the simultaneous operation of multiple scales in the problem. In this letter, we present a recently developed model for treating multiple scales. We then demonstrate the application of the model to three examples: the deformation of a stepped grain boundary (GB), the interaction of lattice dislocations with GBs and the interaction of cracks with GBs.

Recently, the quasicontinuum method was proposed to allow for a seamless treatment of multiple length scales [2,3]. This mixed atomistic-continuum formulation is based on a finite element discretization of a continuum mechanics variational principle. The finite element method serves as the numerical engine for determining the energy minimizing displacement fields, while atomistic analysis is used to determine the energy of a given configuration. This is in contrast to standard finite element approaches where the constitutive input is made via phenomenological models. The method is successful in capturing the structure and energetics of dislocations.

In this paper we generalize the method to allow for the treatment of interfaces, and show how the formulation allows for the simultaneous treatment of dislocations, material interfaces and cracks. We begin with the recognition that from the microscopic perspective the body may be regarded as a collection of $N$ atoms, the total potential energy of which is given by

$$\Pi = \sum_{i=1}^{N} E_i(\mathbf{r}_1, ... , \mathbf{r}_N) - \sum_{i=1}^{N} \mathbf{f}_i \cdot \mathbf{r}_i$$

(1)

where $\mathbf{r}_i$ is the position of the atom $i$, $\mathbf{f}_i$ is the external force on that atom, and $E_i$ is its energy as would be computed from an atomistic model such as the embedded atom method [4] used here. One of the primary objectives in the formulation of the method is to eliminate the redundant atomistic degrees of freedom associated with the regions of the body far from extended defects and hence subject to displacement fields which are slowly varying on the atomic scale. To achieve the requisite degree of freedom reduction we select $M$ representative atoms from the $N$ atoms ($M << N$), chosen to best represent the energetics of the body, the positions $\mathbf{r}_\alpha (\alpha = 1, ..., M)$ of which serve as the reduced set of degrees of freedom. The body is now divided into disjoint cells such that each cell contains exactly one representative atom. The key energetic approximation is that the energy of all of the atoms in a given cell is the same as that of the cell’s representative atom. The positions of the atoms that are not treated explicitly are obtained by interpolating the nodal values of the displacements using a finite element mesh which is constructed with the representative atoms as the nodal points. (One possible implementation of this strategy in two dimensions is to use the Voronoi polygons [5] surrounding the representative atoms as the cells, and the geometric dual of the Voronoi tiling, the Delaunay triangulation [6], as the finite element mesh.)

Given the scheme described above, the approximate potential energy depends only on the positions of the representative atoms $\mathbf{r}_\alpha$ and can be written as

$$\Pi_{reduced} = \sum_{\alpha=1}^{M} n_\alpha \bar{E}_\alpha(\mathbf{r}_1, ... , \mathbf{r}_M) - \sum_{\alpha=1}^{M} n_\alpha \bar{f}_\alpha \cdot \mathbf{r}_\alpha$$

(2)

where $n_\alpha$ is the number of atoms represented by atom $\alpha$, $\bar{E}_\alpha$ is the energy of that representative atom and $\bar{f}_\alpha$ is the effective force acting on the $\alpha^{th}$ representative atom. In practice, $\bar{E}_\alpha$ is computed in two different ways. When the representative atom is located in a region undergoing strongly non-uniform deformation, $\bar{E}_\alpha$ is computed using the usual atomistic rule in which a given atom is
surrounded by its complement of neighbors and the resulting energy per atom is computed. On the other hand, if the representative atom experiences a slowly varying deformation the energy is still computed atomistically, but with the assumption that its environment is distorted according to the local gradients of deformation. The details of the criteria that dictate which scheme is used will be described elsewhere. The key outcome gained in the implementation of the strategy described above is the incorporation of the relevant atomistic nonlinearity and nonlocality that allows for the emergence of defects such as dislocations and cracks, without the attendant singularities that plague linear elastic analyses, or the burden of many redundant atomistic degrees of freedom.

As in our earlier work with this method, a key criterion to the validity of the model is how well the results of conventional atomistics are recovered in the context of defects of known structure. For the purposes of the present paper, the method must successfully reproduce the known static geometric structures of GBs. As a test of the method, we have examined the structure of a range of GBs in several fcc metals. For the moment, we have confined our attention to symmetric tilt boundaries, using embedded-atom type potentials. The key quantitative tests of the outcome of these calculations are an appropriate reckoning of i) the interfacial energy, and ii) the interfacial structure. An indication of the typical energy differences between the quasicontinuum result and the associated direct atomistic calculation is demonstrated by a $\Sigma 5(210)$ GB in Au where the energy obtained by conventional atomistics ($\sim 676 m J/m^2$) \[7\] and the method described here ($\sim 670 m J/m^2$) are in close agreement. Similarly, in all of the cases we have considered (i.e. $\Sigma 5(210)$ in Al and Cu, $\Sigma 3(111)$ in Al, $\Sigma 99(557)$ in Al, and $\Sigma 21(241)$ in Al, Au and Ni), the atomic level geometry at the interface obtained using the quasicontinuum method advocated here was for practical purposes identical to that obtained using direct atomistic simulation. Consequently, it is of interest to turn the method to the analysis of interfacial deformation.

FIG. 1. Step motion under applied shear stress. Atomic positions associated with stepped twin boundary, illustrating the motion of the boundary perpendicular to the boundary plane as a result of an applied shear stress. (a) Initial configuration. (b) Final configuration after the application of the critical stress.

As an example of such deformation, we consider a stepped twin boundary ($\Sigma 3(111)$) in Al that is subjected to a remotely applied shear stress. It is found that once a certain critical shear stress ($\approx 0.033 \mu$, where $\mu$ is the shear modulus relevant to the orientation of interest here) is attained, the step on the boundary serves as a source for $\frac{\pi}{4}[112]$ dislocations which are swept out along the boundary plane. The consequence of the passing of these dislocations is the net downward motion of the twin boundary shown in fig. 1. One question of importance concerning the type of simulations described above is that of the convergence of the results with respect to both system size and mesh geometry. We have found that altering the system size reveals that the critical stress of $\approx 0.033 \mu$ necessary to move the boundary is reproduced to within $\pm 0.003 \mu$ from one simulation to the next. It is interesting to contrast this stress with a typical Peierls stress for a straight dislocation. For example, in the case of a screw dislocation in this metal, we have found \[8\] that the Peierls stress is $0.00068 \mu$, nearly fifty times smaller than the critical stress for advancing the twin boundary. As another comparison to set the scale of the stress determined here, the stress to induce motion of the twin boundary can be compared with that to operate a Frank-Read source which is $\sigma \approx \mu b / L$, where $L$ is the width of the source \[8\]. In light of this estimate, the stress to induce motion of the twin boundary is of the same order as that to operate a Frank-Read source of width $\approx 35b$ (where $b$ is a typical Burgers vector). Although typical Frank-Read sources are larger than $35b$ and hence operate at even lower stresses, the stress found to stimulate motion of the twin boundary is still significantly smaller than the ideal shear strength, and is another example of the "lubricating" effect of heterogeneities in the motion of extended defects.

Despite the existence of useful continuum models of dislocation-GB interactions, it remains a crucial challenge to uncover the microscopic processes that transpire once the dislocation core is in the proximity of a GB. Our earlier work on simulating nanoindentation \[9\] suggests the possibility of using nanoindentation induced dislocations to probe the interaction between dislocations and a GB. As a model system, we consider a block oriented such that (111) planes are positioned to allow for the emergence of dislocations which then travel to the $\Sigma 21(241)$ GB which waits approximately 200 Å beneath the surface (c.f. figure 2a).

Because of the relatively high stacking fault energy associated with the EAM potentials for Al we used \[10\], the dislocations nucleated at the free surface as a result of the indentation process are produced as rather closely spaced (15Å) Shockley partials. As seen in the left frame in part (b) of fig. 2, the Shockley partials have been absorbed at the GB with the creation of a step at the GB. This geometry can be rationalized on the basis of the underlying displacement shift complete (DSC) lattice \[11\] associated with this symmetric GB. We find that the lattice dislocation $\frac{\pi}{4}[110]$ can be split into two DSC lattice vectors,
\[
\frac{a_0[110]}{2} = \frac{a_0[312]}{14} + a_0[241],
\]

where \(\frac{a_0[312]}{14}\) is the Burgers vector of a GB dislocation parallel to the GB and \(a_0[241]\) is the vector associated with the step.

As the load is increased, a second pair of Shockley partials is nucleated and they are not immediately absorbed into the GB and consequently form a pile-up (c.f. fig. 2). These dislocations are not absorbed until a much higher load level is attained. Due to the lack of dislocation activity in the neighboring grain, it may be concluded that this GB does not aid slip transmission.

In order to investigate the interaction between an advancing crack and a GB, we consider the \(\Sigma 21(241)\) GB in fcc nickel. A crack is initiated in one of the grains by removing a single (111) plane, such that the crack tip is located about 2 nm from the GB. The crack is then loaded by applying the isotropic linear elastic displacement fields for a sharp crack at the mesh boundaries. The load is incrementally increased by scaling the boundary node displacements and allowing the interior nodes to relax to their minimum energy configuration.

Two snapshots of the solution are shown in fig. 3. We show the atoms associated with that part of our finite element mesh that is fully refined to the atomic scale in the immediate vicinity of the crack tip. The surrounding mesh, which extends about 300 nm in each direction, has been removed for clarity. The dots are atomic positions, while the contours reveal displacement jumps across active slip planes, indicating the presence of dislocations. Frame (a) of this figure is the configuration after 4 load steps. The atom labeled “ct” indicates the initial location of the crack tip, and one can see that the crack has begun to propagate towards the GB by cleavage. Light grey slip traces emanating from the GB, such as those labeled “d1” and “d2” show where the stressed GB has emitted dislocations, some of which have been pinned against the edge of the fully refined region. The dashed line running diagonally through the figure indicates the initial location of the GB which moves as a result of the high stresses in the crack tip region. This motion is accommodated by the structural rearrangement of atoms in the left hand grain to lattice sites of the right hand grain due to shearing along atomic planes. The solid line through the figure indicates the location of the GB after migration.

In frame (b) of figure 3, the solution after another few load steps is depicted. Here, the crack has reached the
GB and has been blunted when atoms above the plane of the crack again underwent a shearing deformation. This time, however, the right hand grain shears to match the structure of the left hand grain. The two straight solid lines indicate the new location of the GB. The result of this crack blunting is a significant reduction in the stress levels above the crack, and dislocations such as “d1” and “d2” in the first frame have moved back to be re-absorbed by the GB. Further loading of the crack leads to a continued crack blunting due to shearing of atomic planes along the GB. We have studied other GBs [12], where the crack has deflected and continued to propagate along the GB, in contrast to the crack blunting mechanism described here.

![Image](a.png)  ![Image](b.png)

**FIG. 4.** (a) Driving force (normalized by the elastic constant, $c_{11}$) as a function of position $s$ along the GB (normalized by the lattice constant $a_0$). (b) The same force superimposed on the GB for comparison.

To understand these results, we turn to continuum mechanics which provides the basis for evaluating the energetic origins of GB migration. Such reasoning asserts that the driving force on an interface is given by the jump in the Eshelby tensor across the interface, with this tensor defined as

$$P_{ij} = W\delta_{ij} - u_{k,i}\sigma_{kj}. \quad (4)$$

$W$ is the strain energy density, $u_{k,i}$ is the $k$th component of the gradient in the $i$th component of displacement and $\sigma_{kj}$ is the stress tensor. Within the confines of linear elasticity, we have computed the driving force on the interface by using a conventional anisotropic linear elastic constitutive model in conjunction with the standard finite element method to obtain the fields associated with the crack/GB geometry described above. Once these fields are obtained, the resulting driving force may be obtained by computing the jump in the Eshelby tensor across the interface. If we further assume that the GB migration is proportional to the driving force, the driving force profile may be compared directly with the bowed out geometry as shown in figure 4.

In this letter, we have shown how our mixed atomistic and continuum analyses has been adapted to the treatment of interfacial deformation. Such calculations demanded generalization of the original quasicontinuum formulation to allow for the existence of more than one grain at the same time. As validation of the method, we have computed the structure and energetics of a series of different GBs and found entirely satisfactory correspondence between these calculations and those resulting from direct atomistics. The method has been applied to three distinct problems: deformation of a stepped twin boundary, the interaction between dislocations and a GB, and the propagation of a crack into a GB. The calculations on the stepped GB allowed for quantitative evaluation of the stress to move the GB, while calculations on the crack/GB interaction revealed stress induced GB motion which can be rationalized in terms of the driving force on that interface as implied by the jump in the Eshelby tensor. The advantage of the model presented here over standard atomistic calculations is the significant reduction in the computational effort through careful reduction of the degrees of freedom. For example, the number of degrees of freedom associated with the mesh of figure 2a is about $10^4$, while the same atomistic calculation would have required more than $10^7$ degrees of freedom. This approach allows for the simultaneous treatment of defects occurring over many length scales, ranging from individual dislocations to GBs and cracks.

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