Quasicontinuum models of fracture and plasticity

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Abstract

The development of modeling tools which allow for the simultaneous treatment of scales ranging from Ångstroms to microns has stood out as one of the main challenges in materials modeling. In this paper we discuss a formulation of the quasicontinuum (QC) method that allows for a treatment of internal interfaces, opening the possibility of simulating the interactions of cracks, dislocations and grain boundaries. The model is applied to crack tip deformation and is shown to account for both brittle fracture and crack tip dislocation emission. A key example of the method is the treatment of a crack propagating into a grain boundary which reveals both migration of the boundary and that the boundary is a source for the emission of dislocations. © 1998 Elsevier Science Ltd. All rights reserved.

1. Introduction

Recent interest in the multiple scale modeling of materials has been precipitated in part by the existence of questions in the study of plasticity and fracture which necessitate the consideration of nucleation and interaction of dislocations. In many instances, such questions require an appropriate treatment, not only of the small scale features that owe their existence to the presence of the underlying discrete lattice, but also to the long range interactions which can be successfully captured within a linear elastic framework and are difficult to manage with purely atomistic methods. This poses a challenge to conventional modeling techniques which preferentially select a particular length scale as being dominant.

The thesis of the present work is that in some cases a successful approach to modeling the mechanics of materials must freely range over scales from the Ångstrom to the micron range. In an earlier paper [23], we have introduced the quasicontinuum (QC) method in which it is

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supposed that a conventional continuum mechanics formulation can have its range of applicability broadly extended by incorporating atomistically derived constitutive information. Efforts to extend the scope of the method to allow for the treatment of internal interfaces such as grain boundaries (GBs) required a reformulation of the method as will be shown below.

The present paper outlines the amended logic of our mixed atomistic-continuum scheme in light of the changes that were needed in order to treat grain boundaries (for a detailed discussion see Ref. [20]). As in the earlier formulation, the perspective remains that of removing irrelevant degrees of freedom in a systematic way without at the same time interfering with degrees of freedom where they are needed to capture discrete lattice effects. In general, such a reduction in degrees of freedom cannot be carried out homogeneously throughout the material as is envisaged in many of the decimation procedures of statistical mechanics [13]. Rather, one imagines that the elimination of degrees of freedom must be tied to the local field gradients; thus, more degrees of freedom will be removed where the fields are more slowly varying. This requirement is met in our case via the use of graded finite element discretization.

Our mixed atomistic and continuum scheme will be turned to two problems of the type alluded to above, namely, that of crack tip deformation in the neighborhood of a crack blunted at the atomic scale, and secondly, to the analysis of a deformation involving interfaces. In the latter problem, we consider the interaction of a crack with a GB.

Until recently, most of the effort in fracture mechanics has focused on phenomenological descriptions of material behavior (see Ref. [10] for a review). Dissipative deformation processes around a crack tip were treated using continuum plasticity models, while fracture criteria were inserted into the model based either on the Griffith analysis or via a Barenblatt type of model. While these continuum models have been very successful in describing the fracture of materials, they are incapable of elucidating the precise deformation mechanisms near the advancing crack tip. Only through the inclusion of atomic scale information in modeling efforts can we hope to understand these mechanisms that ultimately conspire to produce the phenomena mimicked by the continuum mechanics approach.

The importance of atomic scale effects in fracture has been recognized for some time, and work to understand atomic scale fracture initially focused on analytic models that included lattice discreteness in an approximate way [24]. Early computer simulations of fracture (see, for example, Ref. [22]) were limited by the available computational power, but lead to significant insight into atomic configurations at the crack tip and the effects of lattice trapping. These early studies also demonstrated the agreement between the Griffith criterion and atomistic simulations of brittle fracture. Lately, advances in atomistic simulation of materials and increases in computational resources have made it possible to simulate fracture processes at the atomic scale for relatively large systems. Approaches to modeling fracture at the atomic scale range from the conceptually simple but computationally challenging fully atomistic approach, to a variety of mixed atomistic/continuum models that include atomistic effects either through some approximate scheme or by embedding an atomistic crack tip region in a bulk continuum.

The first approach, that of full molecular dynamics or lattice statics simulations of fracture, has been pursued by a number of groups [1, 4, 6, 8, 12, 16, 17, 27]. Atomistic simulations of fracture are carried out by building a small crystal with an attendant crack tip and applying a strain rate to the crystal boundaries. The number of atoms in such simulation has steadily been
increasing as computer power allows, from a few thousand atoms in the earlier works to tens of millions of atoms most recently. The challenges in such an approach come both from the huge computational power and storage required to explicitly model millions of atoms, as well as from the need to make sense of the vast quantities of information which result. Simulations of $10^8$ atoms are now fairly routine, but such calculations require the resources of massively parallel supercomputers. While such calculations are an impressive demonstration of advances in computation, the task of extracting an understanding of material behaviour which can be used as a basis for higher level models remains daunting.

Despite the challenges of explicitly treating millions of atomic degrees of freedom, fully atomistic studies of fracture have played an important role in our understanding. First of all, molecular dynamics is a fertile setting within which to document and classify the atomic level mechanisms of fracture. They also provide a highly controlled ‘experiment’ with which to test the validity of analytic models. In some cases, such as in the work of [17] and [6], atomistic models have been used to determine the point where continuum assumptions fail. In other cases, the simulations have shed light on counter-intuitive results that may not have been otherwise revealed. For example, Abraham et al. [1] showed that the preferred cleavage planes in fcc crystals cannot be determined simply from a rank ordering of surface energies.

Perhaps the most frustrating aspect of such large atomistic calculations is that so few of the millions of atomic degrees of freedom do anything especially interesting. It has been shown by a number of atomistic studies (see, for example, Refs. [11] and [6]) that a great many of the atoms around a crack tip respond in accordance with elasticity theory. Yet the storage and book-keeping associated with their degrees of freedom—necessary if a purely atomistic approach is used—consumes a large proportion of the computational time. The motivation for a number of researchers has been this realization that despite the need for full atomic detail near the crack tip, the majority of atoms behave in an elastic fashion. As a result, there are now several modeling approaches which aim to reduce the number of degrees of freedom in atomic scale systems. Some of these models, like that of Kohlhoff et al. [14] and Gumbsch [11], effect this reduction by dividing the problem into two distinct zones, one which is fully atomistic and the other which is modeled using conventional finite elements. Another example is the approach of Zhou et al. [28], Zhou et al. [29] and Schiotz et al. [19]. In this instance, the actual number of atomic degrees of freedom is not changed, but rather a large proportion of the atoms are treated using a linear approximation to their response. These linear atoms, while they are still explicitly modeled, demand considerably less computational overhead than fully non-linear atoms, and hence the approach greatly reduces the calculation time. A third method, and that which will be used here, is the QC method.

These mixed approaches can be used to investigate fracture in much the same way as full atomistics, with the advantage of reduced computational demand. For example, [11] studied brittle cracks in fcc crystal under mixed loading, and was able to compute critical loads to failure for sharp cracks and for cracks with atomic scale blunting at the tip. Zhou et al. [28] and Zhou et al. [29] used their simulations to test analytic models of fracture. They determined that the analytic models were ignoring an important contribution to the energetics of crack tip deformation—namely the energy of the ledge which forms when a crack tip emits a dislocation. Finally, Schiotz et al. [19] showed how atomic scale crack blunting can lead to increased resistance to cleavage along atomic planes and possibly enhanced ductility. In this
work, we examine two cracks in single crystals of nickel. In part, this provides a verification that the QC approach is in agreement with existing results and sets the stage for the more complicated problem of the interactions between cracks and GBs. At the same time we use our simulations to discuss the predictions of continuum-based fracture models.

In all of the fracture simulations discussed to this point, the focus has been on a crack in an otherwise perfect single crystal. While understanding this simplified problem is clearly important to the larger story of material fracture, it does not begin to probe the complex interactions between cracks and microstructure so often observed in experiment [15, 25]. Cleri et al. [5] have studied the problem of fracture when a pre-existing crack lies in the plane of a GB both from the point of view of atomistic simulation and by using a continuum model based on the analysis of Rice [18]. In this paper, we pursue a slightly different problem, and consider the case when a crack, propagating through a perfect crystal, impinges on a GB in its path. We present two different GBs that demonstrate two very different deformation mechanisms, to be described below.

2. Methodology

In earlier work [23], the quasicontinuum method has been shown to be a viable candidate as an alternative to lattice statics for the treatment of the structure and energetics of defects such as dislocations. The basic idea of this earlier treatment is the notion that one can think of an inhomogeneously deformed (and possibly defected) body as a continuum for which the kinematics can be described entirely in terms of displacement fields. Then, rather than supplementing this viewpoint with traditional continuum constitutive models, we instead exploit atomistic analysis as the basis of our determination of the total energy of the body. One of the key advantages that emerges from adopting this scheme is the existence of a multiple well structure to the total energy surface which leads to the presence of dislocations.

In the present paper, we find it advantageous to cast our ideas in a different light following Shenoy et al. [20]. The altered perspective lends itself more easily to the geometric treatment of grain boundaries while remaining essentially equivalent to the earlier description for single crystal problems. Rather than commencing with a continuum outlook we adopt the view that our body is composed of some huge number of atoms $N$, and hence that we must at the onset manage $3N$ degrees of freedom. From the atomistic perspective the total energy can be written as

$$E_{\text{exact}} = E(x_1, x_2, \ldots, x_N),$$

(1)

where $x_i$ are the atomic coordinates. We see that the total energy depends explicitly on the entirety of the atomistic degrees of freedom that are present. However, as a result of the inhomogeneous strain field that is present in the body there are some regions where one can imagine an approximation in which a subset of degrees of freedom can be replaced and the resulting total energy can be written as

$$E_{\text{reduced}} = E(r_1, r_2, \ldots, r_M),$$

(2)

where $r_j$ are the coordinates of the subset of atoms selected to represent the energetics of the

total energy. This allows us to divide the atomistic material into a finite element (FE) network, with our attention focused on the nodes with coordinates $r_j$. We note that the atomistic model is a many-body problem.

With the continuum model, we presuppose that the total energy is

$$E_{\text{exact}} = \sum_{i=1}^{N} E_i(x_i).$$

Clearly, since $E_i(x_i)$ depends on the number of degrees of freedom of the $i$th atom, $E_{\text{exact}}$ is a many-body problem. The QC method [7]

$$E_{\text{reduced}} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} R_{ij} |x_i - x_j|^2,$$

where $R_{ij}$ is the distance between the electron density of the two atoms. This followed historical models of the atom such as the Lennard-Jones radius. This is particularly of interest, of the

$$x_j = X_j + R_{ij}.$$
body (thus, $M < N$). The atoms belonging to this reduced set are referred to as representative atoms. It will be shown below that $E_{\text{reduced}}$ can be determined within the confines of our atomistic model.

For the purposes of our model, we identify the representative atoms at once as nodes within a finite element setting and as a subset of the atomic positions. As with standard finite element (FE) formulations, the nodal positions span a mesh of elements (for the moment we restrict our attention to this two dimensional setting and choose our elements to be three nodded triangles). The degrees of freedom of the system are now the displacements of these atom/nodes with the displacements everywhere else obtained by FE interpolation. We now imagine that the atoms which occupy each node will serve to specify the energy in some sub region of the body in their vicinity. Within the context of this formulation, the total energy of the body can be written as

$$E_{\text{reduced}} = \sum_{i}^{M} n_i E_i$$

Here we have used $E_i$ to describe the energy of the representative atom of the $i$th cell and $n_i$ is the number of atoms within the associated region. Mathematically $n_i$ is a quadrature weight, where the exact lattice sum is replaced by an approximate sum with appropriate weights; physically $n_i$ may be thought of as the number of atoms represented by the representative atom $i$. It is immediately clear that in the limit that we fully refine our mesh (i.e. every atomic site in the model is a node), the weights will all be unity and that our total energy will collapse to $E_{\text{exact}}$.

The computation of the quantity $E_i$ which is the energy of the $i$th representative atom, presupposes an atomistic description that allows for a decomposition of the energy as a sum of individual atom energies, i.e.

$$E_{\text{exact}} = \sum_{i}^{N} E_i.$$  

Clearly, simple schemes such as those founded upon semi-empirical interatomic potentials and many-body potentials all admit such a decomposition. For example, within the embedded-atom method [7], which we have used here, the energy of the $i$th atom may be written as

$$E_i = \frac{1}{2} \sum_{j} \phi(R_{ij}) + f(\rho_i),$$

where $R_{ij}$ is the distance from atom $i$ to neighbor $j$, $\phi(r)$ is the pair potential term, $\rho_i$ is the electron density at the site of atom $i$ and $f(\rho)$ is the embedding energy. The rigorous strategy followed here is to build a crystallite of sufficiently large radius around each representative atom such that the energy of the central atom may be computed given the potential cutoff radius. The geometry of this crystallite is dictated by the local state of deformation. In particular, if we demand the position of the $j$th atom which is a neighbor of the central atom of interest, its position after deformation is given

$$x_f = X_f + u(X_f),$$
where \( u(\mathbf{X}_j) \) refers to the displacement field at the undeformed position of \( \mathbf{X}_j \) of atom \( j \), which may be obtained using the finite element interpolation from the nodal displacements.

The interesting consequences of adopting this strategy becomes evident when examining the limits of very large and very small elements. Clearly, in the fully refined limit, the energy of the representative atom becomes identical to that that would be obtained from conventional lattice statics. On the other hand, for the larger elements, the elimination of degrees of freedom has been bought at a price, namely, the fact that all internal atoms are kinematic slaves of the nodal positions themselves. In particular, once the three nodal coordinates have been specified for the element bounding a particular atom, that atom's position is unequivocally determined. This fact suggests an approximation strategy which reveals the other expected limit of our model. Thus, when a representative atom is experiencing a near homogeneous deformation (i.e. the deformation gradients in the elements surrounding the atom are nearly equal), the energy of the representative atom may be computed from the local deformation gradients. Such atoms which are termed 'local' atoms correspond to the nonlinear elastic limit, and result in a significant computational saving (see Ref. [20] for details).

Once we are capable of determining the total energy of the reduced set of degrees of freedom, their equilibrium configuration can be identified by minimizing this energy relative to the nodal positions using standard solution techniques such as conjugate gradient or Newton-Raphson methods. One subtle feature that arises as a result of the multiple well structure of the total energy as a function of the nodal positions is that the solution can depend upon the initial guess for the nodal displacements. This is typical of schemes that minimize energy at zero temperature. Remaining details of the implementation will appear elsewhere.

3. Cracks in single crystal nickel

In this section, we use the QC method to study the mechanisms of fracture in single crystal, fcc nickel, which is modeled using the interatomic potentials of Foiles et al. [9]. At the crack tip, the inclusion of lattice effects is crucial as it is atomistic processes at the sharp crack tip that give rise to dislocations or the onset of cleavage. On the other hand, the model must be large enough that sensible boundary conditions can be employed. The QC method allows for the application of remote boundary conditions while preserving the atomic scale features that are needed for the explicit treatment of defects.

The goal of these QC simulations is twofold. First, it is of interest to observe the atomic scale deformation mechanisms which occur at the crack tip when the crack is loaded in mode I. Second, it is possible to use the method to compute a number of critical quantities associated with the deformation processes, and compare them to results of other models. We will use the QC method to compute the critical stress intensity factor for either brittle fracture or dislocation emission to occur. This will allow for comparison with models such as Rice's Peierls framework for dislocation emission and the Griffith energy release rate concept, in order to quantify the limitations of these continuum based models.

As a preliminary exercise, we consider two different crack geometries and two different crystal orientations. The geometries we use are the edge crack and center crack depicted schematically in Fig. 1. The crystal orientations, which we shall denote as \( A \) or \( B \), are specified

Fig. 1. Schema of the crystal geometry we use in the analysis and simulation of dislocation emission.

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Table 1

<table>
<thead>
<tr>
<th>Details of sin</th>
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<tbody>
<tr>
<td>Crack</td>
</tr>
<tr>
<td>( A )-edge</td>
</tr>
<tr>
<td>( A )-center</td>
</tr>
<tr>
<td>( B )-edge</td>
</tr>
<tr>
<td>( B )-center</td>
</tr>
</tbody>
</table>
by the crystallographic directions along the $x$ and $y$ axes in this figure. Table 1 provides the details of the crystal orientations and model dimensions used. Note that the cracks we model are not ideally sharp, but have a finite opening corresponding to the removal of one plane of atoms prior to loading. All cracks will be remotely loaded in mode I. In this section, we are interested only in studying a single critical event at a crack tip—either the emission of a dislocation or the propagation of a crack. Hence, the simulations proceed only until such an event occurs.

For each of these cracks, we seek to observe the deformation modes at the crack tip, as well as to quantify the critical load at which either the crack advances or dislocations are emitted. The most natural way to quantify this critical load is by making use of the fracture toughness concept of linear fracture mechanics. As we shall explain below, our loading conditions are such that the boundaries far from the crack tip are held fixed to displacements corresponding to the anisotropic linear elastic solution for a sharp crack. Thus, for each load, the displacements at the boundaries correspond to a certain value of applied stress intensity factor $K_I$. We can therefore compute the critical value of $K_I$ at which either dislocation emission ($K_{IC}^d$) or crack advance ($K_{IC}^a$) occurs. The former can be compared to the continuum based model of dislocation emission put forth by Rice [18] while the latter corresponds to the Griffith fracture toughness of the material for the crystal orientation being considered.

<table>
<thead>
<tr>
<th>Crack</th>
<th>$x$-axis</th>
<th>$y$-axis</th>
<th>$a$</th>
<th>$h$</th>
<th>$w$</th>
<th>$d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$-edge</td>
<td>(110)</td>
<td>(001)</td>
<td>1912</td>
<td>3604</td>
<td>3823</td>
<td>3.52</td>
</tr>
<tr>
<td>$A$-center</td>
<td>(110)</td>
<td>(001)</td>
<td>123.8</td>
<td>3604</td>
<td>1912</td>
<td>3.52</td>
</tr>
<tr>
<td>$B$-edge</td>
<td>(111)</td>
<td>(110)</td>
<td>2601</td>
<td>5735</td>
<td>5203</td>
<td>2.489</td>
</tr>
<tr>
<td>$B$-center</td>
<td>(111)</td>
<td>(110)</td>
<td>101.6</td>
<td>3823</td>
<td>2081</td>
<td>2.489</td>
</tr>
</tbody>
</table>
Table 2
Results of single crystal crack models. Units of \( K_{IC} \) are MPa m\(^{1/2}\)

<table>
<thead>
<tr>
<th>Crack</th>
<th>( K_{IC} )</th>
<th>Failure type</th>
</tr>
</thead>
<tbody>
<tr>
<td>A-edge</td>
<td>0.4898</td>
<td>Brittle</td>
</tr>
<tr>
<td>A-center</td>
<td>0.4948</td>
<td>Brittle</td>
</tr>
<tr>
<td>B-edge</td>
<td>0.3956</td>
<td>Ductile</td>
</tr>
<tr>
<td>B-center</td>
<td>0.4611</td>
<td>Ductile</td>
</tr>
</tbody>
</table>

In order to accurately compute \( K_{IC}^0 \) or \( K_{IC}^c \) for a certain geometry, the following strategy is devised. The model is initially set up as either an edge or center crack, as defined in Fig. 1. The mesh is fully refined in a small region surrounding the crack tip (or tips), and gradually coarsens as the distance from the crack tip grows. This mesh design allows for very large models, where the boundaries are always more than 1000 Å from the crack tip. Based on the large model size, it is assumed that the fields at the boundaries can be well approximated by those from linear elasticity, and thus at each load step the boundary node displacements are fixed to these fields. Even for a crack of small but finite width (on the order of a few Å), the large model size allows us to assume that the boundary sees an ideally sharp crack. Hence, a given level of boundary displacement corresponds to a certain value of the stress intensity factor \( K_i \).

The critical value, \( K_{IC} \), at which inelastic deformation (i.e. either crack advance or dislocation activity) occurs can be computed by gradually increasing the displacements at the boundaries according to the linear elastic result, and allowing the internal nodes of the model to relax with each load step. This calculation examines the atomic scale mechanisms whereby the critical stress intensity factor may be seen as a material parameter. The results are summarized in Table 2, where it is seen that for orientation \( A \), the critical stress intensity factors for cleavage are nearly identical. By way of contrast, the orientation for which we find dislocation emission yields different results for the two different geometries. It was pointed out by Gumbsch [11] that while the anisotropic elasticity solution used in this procedure is exact for crack orientation \( A \), it is only an approximation for orientation \( B \). This is because the elasticity solution requires that the coordinate planes coincide with planes of elastic symmetry, a requirement that is not satisfied in orientation \( B \). It appears that our approximate treatment of the elastic fields contaminates our numerical results for the critical stress intensity factor in orientation \( B \).

Fig. 2 shows the atomic failure mechanisms for the edge cracks. Contours in the figure are of slip along active crystallographic planes. For each element, the three planes defined by each pair of nodes are considered, and the maximum of the slip on these planes is plotted. Failure of the center cracks occurred in exactly the same way as for the edge cracks, with the two crack tips behaving symmetrically. The results in Fig. 2 show the crack tip for a load just below the critical load, as well as for a load just above the critical value. In orientation \( A \) we see the crack responds in a brittle manner, as the crack advances into the crystal. On the other hand, orientation \( B \) responds in a ductile fashion, and the crack tip is blunted by the emission of two Shockley partial dislocations normal to the crack face.

As alluded to in Section 2, toughness is an important material property. This toughness makes it a good parameter to test in this approach...
As alluded to above, the cornerstone of linear fracture mechanics is the concept of the fracture toughness, \( K_{IC} \) (see, for example, Ref. [15] for a discussion). The idea that the fracture toughness is a material parameter, independent of the crack geometry or loading conditions, makes it a powerful predictive tool in design. By computing \( K_{IC} \) for a simple geometry, the value can then be used for more general situations. Our calculations provide a means to justify this approach from an atomistic perspective. We see from the results in Table 2 for orientation
A, the values of $K_{IC}$ computed from the edge crack and center crack differ by only a few percent, supporting the claim that $K_{IC}$ is independent of crack geometry.

These results also make possible comparisons to analytic continuum models that seek to describe the same critical values. For crack orientation $A$, we observed that the crack propagated at $K_{IC} = 0.4898 \ MPa \ m^{1/2}$ for the edge crack and $K_{IC} = 0.4948 \ MPa \ m^{1/2}$ for the center crack. This can be compared to the Griffith criterion, which states that for brittle materials, the crack will grow when the energy release rate, $G$, is equal to twice the surface energy, $\gamma_s$, of the newly created faces. The (001) surface energy is computed using the appropriate EAM potentials. Making use of the relationship between $G$ and $K$ (see Ref. [21]), we can convert $G = 2\gamma_s = 3.1406 \ J/m^2$ to $K_{griff} = 0.4752 \ MPa \ m^{1/2}$, which compares well with the values of $K_{IC}$ for the cracks in orientation $A$. This excellent agreement with the Griffith model is to be expected, given that the crystal is perfectly brittle in this case, with no plastic flow occurring [see Fig. 2(b)]. Thus, all of the elastic energy which is released when the crack advances goes into the creation of the new (001) crystal surfaces.

For crack orientation $B$, we can compare the values of $K_{IC}$ at which the dislocation nucleates to that obtained by the approximate method of Rice [18]. The approach of Rice [18] leads to a critical energy release rate in the range of $G = 1.2021 - 1.3745 \ J/m^2$, depending on the value chosen for Poisson’s ratio in this isotropic analysis. These values were obtained using the relaxed unstable stacking fault energy appropriate for this material. Even by choosing the largest of these energy release rates, the equivalent $K_{IC}$ is found to be $K_{IC} = 0.3039 \ MPa \ m^{1/2}$ which is 25% less than the values reported in Table 2. This observation is consistent with the observation of other authors (for example, see Ref. [28], who have noted the tendency of the Rice model to underpredict critical loads to emission. In addition to considering the Rice model of emission, we can compute the value of $K_{griff}$ for this orientation, which should be much higher than the value of $K_{IC}$ at which emission occurred. Indeed, for this orientation $K_{griff} = 0.4823 \ MPa \ m^{1/2}$, a value too high for brittle failure to occur before dislocation emission. The failure of the calculations to predict the same critical stress intensity factor for anisotropic solution used to apply the boundary conditions in this case.

The finite element basis of the QC model makes it easy to compare these results to results based on other constitutive laws. It is of interest to examine the differences between atomistic calculations and linear elastic results. We have made such a comparison by using linear elasticity to model one of our edge crack geometries with the same mesh of constant strain triangular elements as was used in the QC solution, but now with an anisotropic linear elastic constitutive law. The use of identical meshes and elements ensures that errors in the solution due to mesh effects are the same for both the QC and linear elastic result, and therefore will not affect our comparison of the two solutions. Our linear elastic solution was obtained using the commercial finite element code ABAQUS. The comparison is made in Fig. 3 for crack orientation $A$ and $K_l = 0.4896 \ MPa \ m^{1/2}$, corresponding to a load just below the critical load for crack propagation. The contours in this figure correspond to the difference in the strain fields obtained from the two solutions. Note that this is a plot of, for example, $\epsilon_{xx}^{QC} - \epsilon_{xx}^{LE}$. This is the amount by which the strain that occurs in the atomistic model differs from the strain of the linear elastic model, and can be thought of as the strain that is missed by using the linear elastic constitutive model. Because the elements are constant strain triangles, nodal values of

Fig.
Fig. 3. Plots of the difference in strains between the linear elastic and quasicontinuum models.
strain are computed by averaging over all elements that a node touches. It is these nodal strains that are compared in the figure.

The plots suggest that the linear elastic fields are actually quite representative of the QC result, up to a small region near the crack tip of only about 10 Å in radius. Such good agreement between atomistic and linear elastic models suggests that the non-linear zone surrounding an atomic scale crack tip is surprisingly small. Non-linear effects become significant only very close to the tip of the crack. However, it is clear that because the critical event occurs due to the breaking of bonds at the crack tip, an accurate characterization of the non-linear region is essential.

In the non-linear region, strains along the crack faces, $\epsilon_{xx}$, and shear strains, $\epsilon_{xy}$, are still very close to the linear elastic estimate. Only for the three or four atoms right at the crack tip does the shear strain in the atomistic result differ significantly from the linear elastic model, reaching a maximum difference of about 4%. The important non-linear effect is in the strains normal to the crack faces, $\epsilon_{yy}$. Ahead of the crack tip, there is as much as 10% additional tensile strain due to non-linearity. Prior to fracture, the state of stress ahead of the crack tip is close to a state of uniaxial tension, with strains significantly greater than those predicted by the linear elastic model. Meanwhile, the negative values of $\epsilon_{yy}^{QC} - \epsilon_{yy}^{LE}$ in the wake of the crack indicate that the linear elastic solution overpredicts the tensile strains in this region.

4. Grain boundary migration due to the approach of a crack

A more challenging problem that is well suited to the QC approach, is the interaction between a crack and a grain boundary. As an example of this problem, we consider the $\Sigma = 21(421)$ symmetric tilt boundary in nickel, which has a [112] tilt axis and a tilt angle of 44.41°. A crack is initiated in the model by removing a single (111) plane from one of the grains. The initial mesh is shown in Fig. 4, with a close-up of the fully refined crack tip region in the inset. A load is applied at the model boundaries according to the mode I, isotropic linear elastic crack tip fields. The use of the isotropic solution is necessary because the analytic solution for the crack tip fields near an oblique plane of moduli discontinuity is not known. Since our model is neither isotropic nor homogeneous, this approach will not provide any quantitative information about stress intensities or energy release rates. The scheme is merely a convenient method of loading the model. Ten load steps were computed, the first being one for which the external load was zero. This first step was necessary to allow the GB to relax to its equilibrium configuration before the approach of the crack.

Fig. 5 shows the atoms in the fully refined region for various load steps. The loading is quasi-static, and the time parameter in each frame is used to indicate the relative magnitude of the loads, as each load step corresponds to the same increment in boundary displacements. Contours between the atoms are a measure of the displacement jumps across these planes and correspond to the presence of dislocations. Frame (a), at $t = 0$, shows the unloaded crack and GB, and the resulting relaxations. At this point, the GB has rearranged to its minimum energy configuration, and the crack tip has partially closed due to atoms across the crack plane attracting one another.

In frame (b) of incipient propagation, the GB is shown. A load equal to the yield stress of 400 MPa was then applied, resulting in a second propagation. The two on the GB is shown. The propagation of the stacking fault and the Shockley partials are shown with the GB in the second frame. At $t = 4$, the crack has propagated along the GB plane. This propagation is expected to continue in the field of view.
these nodal displacements.

However, it should be noted that the QC model is limited in its ability to capture the full complexity of real crack propagation. The QC model assumes that the crack tip is subjected to a uniform stress field, which is not always the case in real materials. Additional complexities such as the presence of defects, the texture of the material, and the orientation of the grain boundaries can significantly affect the crack propagation behavior.

In frame (b), we move to \( t = 2 \), where we see the first rudiments of plastic flow, as a number of incipient dislocations form along the GB, the most prominent of which is indicated by the arrow. In addition, the left hand grain begins to transform and atoms along the GB rearrange to match the lattice of the grain on the right.

In the next frame, at \( t = 3 \), three fully formed dislocations have traveled away from the GB. The two on the left are Shockley partials, and the region between each partial and the GB is a stacking fault. The EAM potentials used in this simulation exhibit an unrealistically low stacking fault energy, and thus the energetic cost of these faults is small. Meanwhile, a Shockley partial on the right has run up against the end of the fully refined region, and as a result a second partial has been emitted along the same plane.

At \( t = 4 \), the crack starts to propagate towards the GB by the separation of two (111) planes. This is evident in frame (d), where the original crack tip atom is denoted by 'ct'. In addition, more dislocations have been emitted from the GB, the most prominent of these are labeled 'd1' and 'd2'. At this time, the transformation of the left hand grain is substantial, so
can only have either the crack tip on one side of the GB or the other. Notice the grain boundary just below the lower left corner in the GB after the transformation.

The large number of dislocations and transformed regions in this simulation show that the transformed regions have propagated into the GB.

It is interesting to note that the simulations presented by Balluffi [26] show that the grain boundaries are not as effective in the experiments as they are in the simulations. These previous studies show that angle GBs are not effective in preventing crack propagation.

5. Intergranular Crack Growth

As a second example, we present a simulation of crack growth in nickel. The nickel was modeled using a 3D lattice mesh design with a complex crystallographic structure. The loading mechanism was applied along the orientation, and the crack propagated under a constant load. While a driving force was applied, the crack propagated in a linear fashion. The crack propagation was observed at various points, and the crack tip was observed to move at a constant rate.

Despite the complexity of the nickel structure, the crack propagation was observed to be similar to that observed in other fcc materials. The crack propagation was observed to be more or less straight, with the crack tip moving at a constant rate.

While it may seem that the crack propagation is straightforward, the observations,
can only happen above the crack plane, and the result is a discontinuity in the GB at the crack. The new location of the GB can be seen by tracing atomic planes from one grain into the other. Note also that the dislocations above the crack in the left grain are re-absorbed by the GB after the crack blunts, suggesting that the stresses in the region have been reduced to below the level required to sustain the dislocations.

The large stress reduction at \( t = 5 \) means that the next two load steps are unremarkable. The transformation of the left hand grain below the crack continues, while a number of new dislocations form. It is not until \( t = 8 \), which is shown in frame (f), that the crack blunts further. Here, the crack opens by shearing up along the GB. The opening of the crack is accommodated by additional transformation and restructuring of the GB. Beyond \( t = 8 \), the transformed portion of the GB begins to reach the ends of the fully refined region, and the simulation must be stopped.

It is interesting to note the similarities between the grain boundary migration observed in this simulation and that observed in the experimental observations of Würschum and Balluffi [26] and Babcock and Balluffi [2]. While the nature of the driving force is very different in the experimental situation, the mechanisms of boundary migration which were proposed by these previous authors are very similar to those observed here. Specifically, the motion of high angle GBs seems to take place via the shuffling of atoms across the interface.

5. Intergranular fracture

As a second example, we study the interaction between a crack and the \( \Sigma = 5(120) \) boundary in nickel. The tilt axis of the boundary is the [001] direction, and the tilt angle is 36.87°. The mesh design is very similar to that of the previous example, adjusted for the new crystallography, and the crack is initiated by removing a (110) plane from one of the crystals. The loading program is identical to that of the previous example. For comparison with the results of Fig. 5, the same load steps are shown for the new model in Fig. 6. The differences in the behaviour are immediately apparent. Due to the lack of available slip systems in the new orientation, there is no dislocation activity during the simulation. The crack propagates to meet the boundary, but note that the boundary does not migrate as in the previous example. While a driving force exists on this boundary as well, it is not high enough to lead to boundary motion. When the crack reaches the boundary it branches, running down along the boundary as well as up into the right grain, dragging the GB along and leaving in its wake a region where the right grain has transformed to match the crystallography of the grain on the left.

Despite the results of these calculations, intergranular fracture is not observed experimentally in fcc nickel [3]. The fact that we see this behaviour in our simulations may be explained by a number of approximations in our model. First, the fact that our model is not fully three dimensional constrains certain deformation mechanisms that would be readily accessible to real materials. Secondly, our simulation is done at zero temperature, which makes the material more likely to behave in a brittle fashion. Finally, it is possible that the EAM potentials themselves are not able to accurately describe the GB structure and energetics.

While it may be difficult to make direct contact between this simulation and experimental observations, the differences between Figs. 5 and 6 demonstrate the ability of the QC model to
models of crystalline materials, we allowed us to see the effects of the grain spacings from the simulations.

In studying the simulation, one of the most interesting features was approaching the grain boundary activating a secondary crack is accommodated. Finally, the crack tip accommodated an additional crack.

For the simulations, we used a reduced dimensionality to allow boundary and the crack to interact.

The quasi-continuum approach to the fracture mechanics, we used the use of realistic models with full atomic scale, even when the deformation is not directly associated with the rules.

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References

models of crack tip plasticity like that proposed by Rice [18]. In addition, the model has allowed us to examine the importance of non-linear effects near a crack tip. The results indicate that linear elastic analysis is quite representative of the fields, up to only a few lattice spacings from the crack tip.

In studying the interaction between cracks and grain boundaries, we have revealed a number of interesting deformation mechanisms. In the example of the \( \Sigma = 21(421) \) boundary, the approaching crack induces the GB to migrate towards the crack tip, at the same time activating a number of dislocation sources along the boundary. As a result, the advance of the crack is accompanied by a significant amount of plastic flow originating from the boundary. Finally, the advance of the crack is arrested as it is blunted by the boundary, a process that is accommodated by GB sliding.

For the \( \Sigma = 5(120) \) boundary, the lack of any available slip systems (due in part to the reduced dimensionality of our model) leads to intergranular fracture. The crack reaches the boundary and then branches, moving along the boundary in one direction and up into the neighboring grain in another direction.

The quasicontinuum method presented in this paper provides a practical tool for simultaneously modeling multiple length scales. This approach is important in understanding fracture mechanisms, as atomic level detail can be included at the crack tip while still making use of realistic boundary and loading conditions at larger scales. In addition, the inclusion of full atomic detail in the vicinity of the crack tip allows for a true characterization of the deformation processes. Fracture, plasticity and grain boundary migration are all automatic consequences of the discrete lattice, eliminating the need for \textit{ad hoc} fracture criteria or flow rules.

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References


Abstract

In this paper, we present a new computational approach for simulating the fracture of concrete, including the simulation of the complex behavior of the concrete matrix and the deformation of the aggregate particles. We validate our approach by simulating a single edge notched beam (SENB) and comparing the results against experimental data. The model is able to capture the softening behavior of the concrete and the propagation of cracks, which is a key feature of the material.

The model is implemented using a high-performance computing environment, and the results are presented in a clear and concise manner. The approach is expected to be useful for understanding the behavior of concrete in various applications, such as in the design of structures and in the study of material science.