Quasi-Atomistic Models of Fracture and Plasticity

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Abstract

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 reformulation of previous work on the quasicontinuum method that allows for a treatment of internal interfaces. The model is applied to deformation at a blunt crack tip and to the interaction of dislocations with a grain boundary.

Keywords

Quasicontinuum, dislocation nucleation, finite-elements, atomistic.

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 the long range interactions which can be successfully captured within a linear elastic framework and are difficult to manage with purely atomistic methods. Many problems like those mentioned above pose challenges 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 at least the Ångstrom to the micron range. In an earlier paper (Tadmor, Ortiz and Phillips 1996), we have introduced the quasicontinuum method in which it is supposed that a conventional continuum mechanics formulation can have its range of applicability broadly extended by incorporating atomistically derived constitutive information. Efforts to enlarge the scope of the method to allow for the treatment of internal interfaces such as grain boundaries 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 Shenoy, Miller, Tadmor, Phillips and Ortiz 1996). 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. 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 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 deformation involving interfaces. In the latter problem, we consider the interaction of dislocations with a grain boundary.

Methodology

In earlier work (Tadmor, Ortiz and Phillips, 1996), 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 which can be described kinematically entirely in terms of displacement fields. However, 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, Miller, Tadmor, Phillips and Ortiz (1996). 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 outset manage $3N$ degrees of freedom. From the atomistic perspective the total energy can be written as

$$E_{exact} = E(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N), \tag{1}$$

where $\mathbf{x}_i$ 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

$$E_{reduced} = E(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_M), \tag{2}$$

where $\mathbf{r}_i$ are the coordinates of the subset of atoms selected to represent the energetics of the body (thus, $M < N$). The atoms belonging to this reduced set are referred to as *representative* atoms. It will be shown below that $E_{reduced}$ can be determined within the confines of our atomistic model.

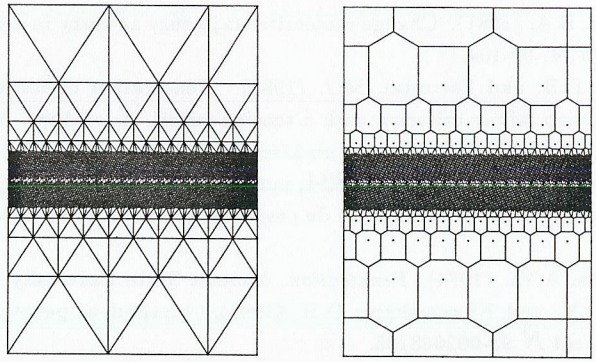

Figure 1: Voronoi diagram and finite element mesh for the $\Sigma 7$ boundary. Each vertex in the figure on the left is a node (or representative atom). These nodes are used to represent all the atoms within their Voronoi polygons, as shown on the right.

For the purposes of our model, we identify the $\mathbf{r}_i$'s at once as nodes within the finite element setting and as a subset of the atomic positions. As within typical finite element formulations, the nodal positions span a mesh, the various polygons of which are the elements (for the moment we restrict our attention to this two dimensional setting and choose our elements to be three noded triangles). The system degrees of freedom are now the displacements of these atom/nodes with the displacements everywhere else obtained by FEM 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, in particular, by determining the geometric dual to the finite element mesh itself (that is, by surrounding each representative atom by its associated Voronoi polygon). For the purposes of illustration, in fig. 1 we show the finite element mesh and associated Voronoi tiling that arises in a model of a $\Sigma 7$ grain boundary. Within the context of this formulation, the total energy of the body can be written as

$$E_{reduced} = \sum_{i}^{M} n_i E_i. \tag{3}$$

Here we have used E_i to describe the energy of the representative atom of the i^{th} Voronoi cell and n_i is the number of atoms within the associated Voronoi polygon. 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), each Voronoi polygon will only contain one atom and that our total energy will

collapse to E_{exact}.

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

$$E_{exact} = \sum_{i}^{N} E_i. \tag{4}$$

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 (Daw and Baskes 1983), which we have used here, the energy of the i^{th} atom may be written as

$$E_i = \frac{1}{2}\sum_{j} \phi(R_{ij}) + f(\rho_i), \tag{5}$$

where R_{ij} is the distance from atom i to neighbor j, $\phi(r)$ is the pair potential term, ρ_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

$$\mathbf{x}_j = \mathbf{X}_j + \mathbf{u}(\mathbf{X}_j), \tag{6}$$

where $\mathbf{u}(\mathbf{X}_j)$ refers to the displacement field at position $\mathbf{X}_j$, 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 savings (see Shenoy, Miller, Tadmor, Phillips, Ortiz (1996) for details).

Once 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.

Illustrative Examples

As mentioned above, the quasicontinuum method has already been successfully applied to a range of problems involving dislocations. In this paper, we describe two more recent applications. One problem of abiding interest is that of crack tip deformation and the plastic deformation that attends it. A host of recent work, both analytic and computational, has been directed at setting up criteria that can distinguish between the propensity of an atomically sharp crack to emit dislocations and thereby blunt, or alternatively, to cleave (see Schiotz, Canel and Carlsson (1996), Gumbsch (1995), Rice (1992)). Though most such models make the limiting assumption of reduced dimensionality, as we do here, such models may still serve as a testbed for the analysis of key questions such as whether or not linear elastic analyses can shed any light on such small scale phenomena, and how changes in crystal orientation and material parameters alter the inclination toward a particular type of deformation.

One of the areas of particular interest of late has been that of the role of blunting in inhibiting subsequent dislocation emission or cleavage. To investigate this question, we have carried out calculations on fcc Ni using the same embedded-atom potentials as those favored by Gumbsch (1995). As part of our analysis, it is imperative to allow for the mesh to refine in response to the presence of severe deformations such as are anticipated at the crack tip. As in our earlier work, the criterion that triggers mesh adaption is a simultaneous evaluation of the second invariant of the Lagrangian strain tensor and the energy associated with a given element. Our model is well suited to crack problems, which typically require large simulation geometries despite the fact that all of the non-linear deformation remains highly localized near the crack tip. The degree of freedom reduction resulting from our model allows us to simulate blocks of atoms as large as $0.5\mu m \times 0.5\mu m$ on a DEC Alpha workstation, with each load step requiring less than an hour of CPU time.

Preliminary calculations on blunt crack geometries have exhibited both dislocation emission and crack propagation processes depending on the crystal orientation, initial crack tip geometry, and atomic potentials. However, the solution procedure is indeed subtle and we have noted that entirely different deformation outcomes are possible depending upon the size of the load step used. As an example of these preliminary calculations, consider fig. 2 where we show a close-up of a blunt crack subjected to mode I loading. The full mesh is approximately $0.5\mu m \times 0.5\mu m$, and at the boundaries we apply the linear elastic crack tip field displacements. Like in the earlier work of Gumbsch, 1996, we see that this crack initiates an atomically sharp crack at its tip, which propagates into the crystal. Because the crack tip region is fully refined and non-local, all atoms in this region are explicitly included in the energy calculation, and the energy of the newly created surfaces of the sharp crack is implicitly accounted for.

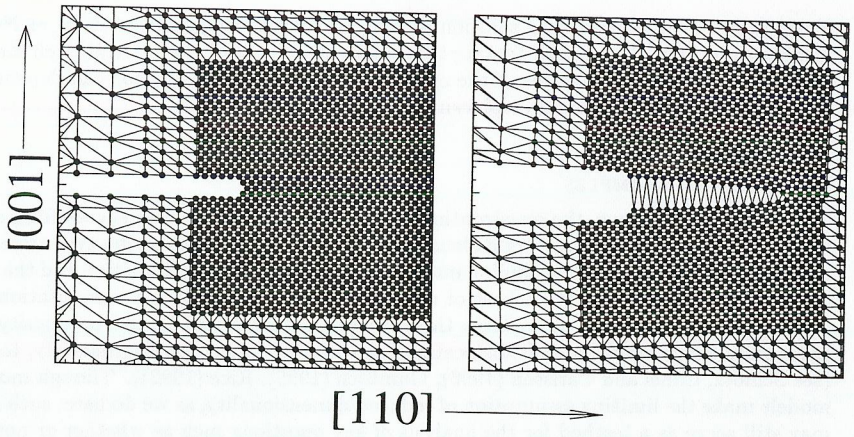

Figure 2: A sharp crack propagating from the tip of a pre-existing blunt crack in fcc nickel. The figure on the left is the unloaded crack tip. The figure on the right is the crack after several load steps have been applied.

Deformation in materials is invariably tied to the behavior of interfaces. Another area in which the method described here might serve to yield insights distinct from those rendered possible by conventional analyses is in the study of grain boundaries. Of particular interest are questions concerning how grain boundaries migrate in response to defects present in the interfacial structure itself, and secondly, how do such boundaries control the transmission of slip between adjacent grains. In particular, we have chosen to study the interaction of dislocations with a grain boundary in aluminum (embedded atom potentials developed by Ercolessi and Adams (1993) were used). The dislocations are generated by indentation on the free surface and on nucleation, travel towards the grain boundary. The first frame of fig. 3 shows the snapshot of the atomic positions immediately after the initial nucleation of two Shockley partials. It is seen that one of the partials is absorbed into the boundary and a step forms on the boundary. The second partial is subsequently absorbed following a slight increase in applied load. On continuing the indentation another pair of Shockley partials is nucleated and they form a pile-up ahead of the boundary as is seen in the second frame of fig. 3. This pair of dislocations is later absorbed at a higher level of stress produced by further indentation.

Conclusion

Preliminary work in a number of different areas such as the static structure and energetics of extended defects such as dislocations and grain boundaries and the analysis of

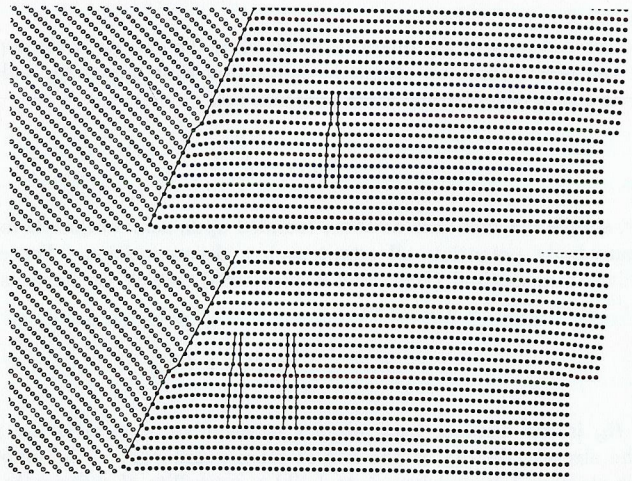

Figure 3: Interaction of dislocations with a $\Sigma 7$ grain boundary.

deformation-induced plasticity suggest that the mixed atomistic and continuum scheme presented here provides a viable alternative to traditional lattice statics allows for the treatment of multiple scales simultaneously. Here we have shown how the method may be turned to two issues of importance in the attempt to include nanoscale understanding into plasticity and fracture. First, we have seen that crack tip deformation may be conveniently evaluated with these methods, with crystal symmetry treated naturally. Secondly, we have seen how the quasicontinuum framework may be turned to the question of slip transmission at interfaces.

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