Mixed Atomistic and Continuum Models of Deformation in Solids

E. B. Tadmor and Rob Phillips

Division of Engineering, Brown University, Providence, Rhode Island 02912

Graduate Aeronautical Labs, California Institute of Technology, Pasadena, California 91125

Received October 17, 1995

The modeling of processes involving multiple length scales is an area of pressing concern, especially in problems such as nanoindentation and crack tip dislocation activity. In these cases, there is more than one characteristic dimension with the nanometer scale arising due to the presence of extended defects such as dislocations and a second length scale at least 2 orders of magnitude larger set by the scale of the indenter or the crack tip itself. To properly model such processes, both scales must be treated explicitly, which is normally beyond the scope of conventional atomistic and continuum analyses alike. This paper describes a quasicontinuum method which seizes upon the strengths of both atomistic and continuum techniques and allows for the simultaneous treatment of multiple scales. The method is based upon a continuum formulation of the problem of interest as a boundary value problem treated within the confines of the finite element method. We part company with traditional approaches by utilizing direct atomistic calculations as the source of the constitutive input used in the finite element analysis. The method is illustrated through application to the case of the structure and energetics of single dislocations. This case is a stringent test as it represents an extreme limit for the model since dislocation core structures are primarily dictated by lattice effects. It is then shown how the method may be applied to problems of tribological concern such as nanoindentation, where it is found that dislocations are initiated beneath the indenter.

I. Introduction

The ultimate aim of the modeling of materials is not only to understand the mechanisms which govern processes such as nanoindentation but eventually to predict and control them. A criterion for successful modeling of these processes must include the ability to model both the complex geometries and loading conditions encountered in a variety of experiments. Further, the model must reflect the subtle distinctions that separate the properties of one material from the next.

One of the difficulties in the modeling of tribological processes such as contact is the presence of multiple length scales, none of which can necessarily be singled out as the dominating influence in governing the system's behavior. On the one hand, much of the material can be successfully treated as a linear elastic medium, making it grossly inefficient to carry out direct atomistic simulation in such regions. By way of contrast, the plasticity inherent in nanoindentation processes, for example, is carried by discrete numbers of dislocations. A recent experimental analysis of indentation in Fe–3 wt % Si single crystals by Gerberich et al.† indicates that for an indenter of tip radius 66 nm and indentation depths of between 6 and 26 nm, roughly 15–70 dislocations can be impugned as the primary carriers of the resulting plasticity. These dislocation densities are sufficiently low as to defy a treatment via conventional continuum plasticity and appear to demand an explicit treatment of the dislocation degrees of freedom.

From the standpoint of modeling, these issues pose competing resolution demands. As a result, it is of interest to build models that can seamlessly make the transition from the regions well described by continuum mechanics to those demanding explicit treatment of the lattice degrees of freedom. A second point concerning the development of such models is that it is desirable to ensure that the constitutive input is as faithful to the underlying atomistic mechanisms as possible. One modeling approach is that of direct atomistic simulation. Here, each and every atomistic degree of freedom is explicitly accounted for, and the minimum energy configuration is determined on the basis of interatomic interactions. While such numerical experiments are a powerful tool for providing insights into the mechanisms responsible for a given process, they are cumbersome and leave a desire for more concrete insights. The trend toward simulating ever larger systems (with the present record somewhere in the neighborhood of 10^7 atoms) leaves us faced with the daunting bookkeeping task that statistical mechanics was formulated to eliminate.

An alternative perspective for the modeling of such systems is on the basis of continuum models. Such models often admit of elegant analytic solutions for highly idealized geometries, and these solutions are often instructive in guiding intuition concerning more complex geometries. Further, continuum models are routinely solved numerically via methods such as the finite-element method. One problem with these models, especially for those involving plastic deformation, is that they are founded upon phenomenological constitutive models which are an idealization of observed deformation properties.

There have been a number of models, which have met with varying degrees of success, whose aim is to combine the atomistic and continuum approaches. One class of...
such models is built around the idea of linking the atomistic region to the continuum via a special set of transition region boundary conditions. These models have led to interesting observations on problems such as crack tip dislocation nucleation. An alternative viewpoint, and the one adopted here, aims to build a seamless model in which the formulation remains a standard continuum mechanics boundary value problem with the added feature that the constitutive properties of the continuum are drawn directly from atomistics.

Constitutive relations remain, in some sense, the Achilles heel of continuum formulations. The constitutive statement related to a given boundary value problem must remain an external phenomenological input into that problem. In many cases, there is resounding experimental evidence that stands behind the particular choice of constitutive model, with linear elasticity serving as the prototypical example. However, whenever selecting a constitutive model, there is always the danger of a priori constraining the system to a mode of deformation that may not be the actual preferred physical mechanism. Ultimately, constitutive relations can be thought of as arising from the playing out of mechanistic features either at the atomistic or at microstructural scale. Because of powerful recent advances in the use of atomistics to determine parameters ranging from elastic constants to activation energies for transport processes such as self-diffusion, it is an opportune time to reexamine the ways in which microscopic calculations can be used as the explicit basis of constitutive phenomenology.

II. The Quasicontinuum Method

Continuum mechanics is founded on the idealization of a material as a continuous distribution of a variety of field variables such as strain and temperature. For problems in the mechanical properties of materials, the continuum statement of the problem often centers on satisfying the equilibrium equations which may be written as

\[ \sigma_{ij,j} = 0 \]  

(1)

where summation over repeated indices is implied and \( \sigma_{ij} \) are the elements of the stress tensor. The equilibrium equations must be supplemented by the relevant boundary conditions which put requirements upon the displacements and/or forces on the body's surface. A convenient numerical basis for solving these problems is to advance a variational statement of the equilibrium equations and to implement the finite-element method in which the continuum is discretized by a geometric tiling, the vertices of which are known as nodes and for which the unknown displacements must be determined. The displacement and other fields of interest are then found elsewhere via interpolation. In conventional finite-element formulations, the material response is included on the basis of the type of constitutive relations discussed above. For example, in a linear elastic material, the stress and strain are related by the familiar generalized Hooke's law,

\[ \sigma_{ij} = C_{ijkl} \varepsilon_{kl} \]  

(2)

where \( C_{ijkl} \) is the elastic modulus tensor and \( \varepsilon_{kl} \) is the small strain tensor. Often, such constitutive phenomenology is based upon the existence of a few material parameters (the elastic moduli, diffusion constants, thermal expansion coefficients are a few representative examples) which serve to specify the constitutive response completely.

However, as noted above, in many cases, the constitutive response is the direct result of microscopic processes that admit of explicit specification. The quasicontinuum method parts company with traditional finite element formulations in that the constitutive input is drawn directly from calculations at the atomic scale. In Figure 1, a schematic representation of the discretized continuum is shown, indicating the way in which the lattice degrees of freedom are joined to those of the continuum. Constitutive information is input into the model at special points within the elements known as quadrature points. The strain energy at these quadrature points is obtained in the quasicontinuum method by selecting a representative atom in the vicinity of this point and computing its energy using atomistics. In its simplest form, the method exploits the so-called Cauchy-Born rule, which is a local approximation, and determines the strain energy at a given point by using the strain energy associated with a crystal subjected to the same homogeneous deformation as exists at that point. For example, if the deformation at a given point in the continuum is described by a deformation gradient tensor \( \mathbf{F} \), then the strain energy is determined from a lattice calculation by deforming the perfect crystal lattice vectors \( \mathbf{A} \) into the deformed set \( \mathbf{FA} \), as shown in Figure 2. The discrete lattice calculation for this homogeneously deformed crystal is performed in our case by computing the energy using the embedded-atom method (EAM)\(^8\) which gives an energy as a function of the atomic positions of the form

\[ E_{\text{tot}} = \sum_i U(\rho_i) + \frac{1}{2} \sum_{ij} \phi(R_{ij}) \]  

(3)

(7) Tadmor, E. B.; Ortiz, M.; Phillips, R. Phil. Mag., in press.
(8) In this work we used the EAM potentials developed by Ercolessi and Adams: Ercolessi, F.; Adams, J. B. Europhys. Lett. 1993, 26, 583.
Deformation in Solids

Figure 2. Illustration of the Cauchy–Born rule which maps undistorted lattice with basis vectors \( \mathbf{A} \) into homogeneously deformed configuration with basis vectors \( \mathbf{FA} \).

Figure 3. Invariance of strain energy upon shear deformation as obtained using atomistic formulation of the constitutive model.

In the EAM format, the energy is a sum of an embedding term \( U \) which is evaluated at the local electronic density \( \rho \) and a pair potential term \( \phi \) which is summed over all interatomic spacings \( R_{ij} \). Thus, the strain energy can be computed at the various representative points in the continuum demanded by the finite element analysis and the stresses obtained straightforwardly via differentiation. One powerful result of this formulation is that the constitutive phenomenology automatically inherits crucial symmetries of the underlying crystal lattice. One crucial symmetry making possible the stable development of dislocations is slip invariance as shown in Figure 3. This figure demonstrates that the energy is a periodic function of the shearing angle, with the periodicity determined by the lattice translations corresponding to the Burgers vector. Though our calculations were performed within the confines of the embedded-atom method, in principle, any microscopic total energy description can be used.

Despite the fact that the Cauchy–Born rule provides the most elegant formulation for inserting constitutive information into the finite element calculations, it suffers from a few key flaws. Most importantly, since the local formulation described above treats all deformation as though the representative atom is at the center of a crystal subject to homogeneous deformation, this analysis is blind to defects that do not admit of such a homogeneous description; defects such as stacking faults, grain boundaries, and surfaces. These shortcomings induced us to develop a nonlocal formulation of the model in which inhomogeneous deformation is treated explicitly. The key idea in this case is to ensure that the representative atom in the element of interest sees a neighbor environment appropriate to the state of inhomogeneous deformation in that atom's vicinity. This requirement is instituted by using the interpolated continuum displacement fields to distort the atom's neighbor environment according to the relation

\[ x_n = X_n + u(X_n), \]

where the subscript \( n \) refers to a particular atom. This equation relates the position of a given atom in the undistorted lattice \( (X_n) \) and its position \( (x_n) \) in the presence of the displacement field \((u(X_n))\). The energy of the representative atom is then computed in exactly the same way as in the local formulation and is used as the basis of the constitutive input for that particular part of the continuum.

Once the continuum has been discretized via the finite-element formulation and the constitutive input has been obtained at the relevant points within the elements (the quadrature points), the solution of the boundary value problem of interest amounts to the determination of the unknown nodal displacements which are related through a series of nonlinear equations which must be solved iteratively.

III. Applications of the Method

One of the central criteria considered in the formulation of this method was the desire for a seamless spanning of multiple length scales. For the types of problems considered here, there are two limiting regimes. At very small length scales and in the vicinity of lattice defects such as dislocation cores and grain boundaries, the discrete lattice effects are dominant. In the opposite extreme, macroscopic deformation is characterized by sufficiently slowly varying fields that conventional continuum methods should apply.

As a first test of the model, it is crucial that in these two extremes limits, the model recovers the well-known results of these regimes. As a test along these lines, we have considered the static dislocation core structures of dislocations in fcc Al. As an illustration of the method in this limit, consider the conventional fcc edge dislocation which glides on \( \{111\} \) planes with a Burgers vector of the type \((a_0/2)(110)\). For these dislocations, the perfect dislocation is susceptible to splitting into two Shockley partial dislocations. For the purposes of testing the model, we have compared the structures for these dislocations that emerge from both the quasicontinuum method and conventional atomistic simulation such as molecular dynamics or lattice statics.

In Figure 4, the results of the quasicontinuum solution for this edge dislocation are shown. In frame a, the finite-element mesh is shown superposed with the out-of-plane displacement field. As remarked in the previous section, the solution to this problem amounts to determining the unknown nodal displacements which, because of the finite-element interpolation, imply a solution for the displacements throughout the body. As a convenience for obtaining geometric insight into the meaning of the resulting displacement fields, these fields can be used to deform the atomic positions associated with the perfect fcc lattice. For example, if we consider the atom in the perfect fcc lattice with position \( X_0 \), then its position after the quasicontinuum solution will be given by the results of eq 4. In frame b, the atomic positions implied by the QC solution for this edge dislocation are shown.

A few key features of this solution are worth noting. First, despite the fact that our initial configuration for the displacement fields corresponded to a perfect edge dislocation, the solution led to a pair of Shockley partials. Secondly, the splitting of these partials, which is dictated by the stacking fault energy, is precisely the value obtained in the lattice statics simulations. Another of the critical specifications for the development of the model was that it be efficient in its handling of the gradients in the...
displacement fields. In particular, for those regions subject to slowly varying fields, it is unnecessary to keep track of all of the lattice degrees of freedom. This specification is fulfilled through the use of mesh refinement. That is, in significantly deformed regions, the mesh will be highly refined with elements with typical atomic dimensions carrying the critical field information. On the other hand, in the regions of little action, the mesh will be coarse. The savings as a result of this procedure are shown in Figure 5. It is clear that the QC method results in a considerable reduction in the number of required degrees of freedom relative to a full atomistic calculation, while at the same time allowing for resolution of the core regions normally forbidden to a continuum formulation.

The significance of the ability of the QC formulation to support stable dislocations is that it now becomes possible to simulate processes such as nanoindentation and crack tip loading, both of which can involve the nucleation and emission of discrete numbers of dislocations in a macroscopic setting.

IV. Quasicontinuum Modeling of Nanoindentation

From the standpoint of modeling, small-scale contact mechanics poses a number of challenges. One of the intriguing features of nanoindentation experiments is that they appear to demand the explicit treatment of multiple length scales. Indenters with a radius of curvature on the order of 50–100 nm can now be used in precise experiments. Analysis of the dislocation activity beneath the indenter leads to the conclusion that the number of dislocations activated by these processes are typically less than 100.

There are a number of issues that must be considered if any model of nanoindentation is to be considered as successful. One such issue is that of the force–displacement relations that are observed as a result of indentation. Can the results of such measurements be predicted with attendant insights into the trends separating the behavior of one material from another? A second area of concern is that of the role of coatings. For example, if a metallic substrate is covered by a thin oxide layer it is of interest to predict the way in which the results for the clean substrate should be amended in the presence of the coating. Another point of interest is the way in which the plastic deformation beneath the indenter is governed by the orientation of the underlying crystal lattice. At a more fundamental level, Sharp, Ashby, and Fleck\(^9\) have formulated deformation mechanism maps for static indentation which divide the indentation response into elastic, elastic–plastic, and brittle regimes. From the standpoint of understanding material trends, it is desirable to determine the ways in which this “indentation phase diagram” is determined by the properties of the atoms of which the solid is composed. All of these questions can potentially be addressed via the quasicontinuum method.

Our preliminary simulations in this area have centered on the analysis of pseudo-two-dimensional models of indentation; we have considered both rectangular punches and rounded indenters. The extension of these methods to consider the fully three-dimensional case, while tempting, is as yet untried and will demand the enhancement of the current models.

of our techniques for establishing an initial mesh as well as its subsequent refinement. Our initial calculations have considered a special crystal orientation in which the Al substrate is oriented such that (111) planes are perpendicular to the face being indented. This orientation was selected since it allows for the development of conventional fcc edge dislocations of the type discussed in the previous section to form directly beneath the indenter.

We have considered two limiting cases which contrast the type of outcomes that may be expected from the simulations. In one limit, the indenter is idealized as a small rigid flat punch of width 23.2 Å. In this case, the sharp indenter corner is unforgiving and leads to the nucleation of dislocations after shallow indents. The opposite limit is more typical of experimental indenters, where we have chosen a wedge indenter with a rounded tip with a radius of curvature of 66 nm.

The rectangular block indentation simulations lead to results such as those shown in Figure 6. Only half the punch and substrate were modeled with symmetry boundary conditions applied at \( x = 0 \). In frame a, we show the fully refined mesh used in this case, after the sample has been subjected to an indentation of 6.4 Å. Superposed on the figure are the out-of-plane displacements that develop as a result of the indentation. In this case, it is clear that the indentation has led to the development of partial dislocations separated by stacking fault ribbons. This claim is substantiated in frame b, which shows the atomic positions implied by the QC solution. The evolution of the dislocation activity beneath the indenter is best captured via a series of snapshots of the types shown in the figure. These simulations represent a first step in using the quasicontinuum method to simulate processes involving multiple dislocations.

One of the challenges in constructing these models is the ongoing mesh refinement that must accompany processes such as dislocation nucleation and emission. As the indentation process proceeds the large strains under the punch trigger automatic mesh adaption which leads to refinement in areas of interest. Then as dislocations nucleate, the refinement follows the paths of the dislocations allowing them to move away from the punch into the substrate. Simulations for the rectangular wedge indenter which implement this adaptive meshing strategy are shown in Figure 7, where it is seen that a wave of mesh refinement accompanies the dislocations as they move down the slip plane. The development of efficient criteria for this adaptive meshing poses one of the next challenges in the development of the quasicontinuum method.
The opposite limit that has been considered is that of the curved indenter. In this case, the response is elastic for indentation depths deeper than those for which the first dislocation was nucleated in the rectangular indenter case. The mesh refinement that has taken place for the rounded indenter after an indentation depth of 4.6 Å is shown in Figure 8. This distinction between the rounded and wedge indenters raises interesting questions about the connection between the indenter geometry and the criterion for dislocation emission. Our preliminary results indicate that the sharp corners in the rectangular wedge indenter lead to dislocation emission at much shallower depths than does the rounded indenter.

V. Concluding Thoughts

Continuum mechanics and atomistic simulation are both fields with well-defined research goals and a history of major successes. Because of experimental developments that now make possible the quantitative analysis of the mechanical properties of materials at the nanoscale, much recent effort has gone into the development of modeling tools that can successfully span between these two extremes. From the standpoint of continuum models, one way in which smaller scales can be considered is through the development of constitutive models that explicitly account for the mechanisms which are known to dictate many mechanical properties.

This paper provides an overview of both the philosophy and details of implementing a mixed atomistic and continuum algorithm for investigating some of the nanoscale phenomena addressed above. The formulation of problems in the mechanical properties of materials as boundary value problems is maintained, as in conventional continuum formulations, but with the proviso that the constitutive input into the formulation of the boundary value problem be drawn from calculations which explicitly account for the interactions between atoms. The advantage of this approach is that the method can at once seize upon the degree of freedom reduction afforded by the continuum method, while inheriting the crucial symmetries (most notably slip invariance) intrinsic to the lattice calculations.

Nanoindentation experiments serve as one example of the type of problem requiring a multiple scale analysis. Preliminary simulations using the quasicontinuum method suggest that the method can capture both the elastic and plastic effects that accompany indentation, holding out the hope of providing an atomistic basis for the types of indentation deformation mechanism maps suggested by Sharp et al. The seamless treatment of multiple scales is one of the key themes associated with the quasicontinuum method, and an example of this treatment is evident in Figure 7 which shows the role played by adaptive mesh refinement in effecting this goal. Some of the issues yet to be confronted in the simulation of these indentation processes is the role of substrate lattice orientation, the way in which chemical impurities will alter the dislocation activity and resulting force-displacement curve, and the role of microstructural elements such as grain boundaries in impeding the motion of dislocations.

Acknowledgment. We are grateful to Dave Embury, Bill Gerberich, Owen Richmond, and V. Shenoy for useful suggestions and comments. This work was supported through AFOSR Grant F49620-92-J-0129 and NSF Grant CMS-9414648.

LA9508912