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Stress and Strain Analysis in Molecular Dynamics Simulation of Solids

Molecular dynamics simulation of solid materials is applied to a two-dimensional indentation problem. Methods are presented for calculating the stress and strain tensors at interior points within the model. The stress calculations corresponding to the elastic deformation portion of the indentation process are compared with an analytical continuum solution. Stress calculations are also presented for the plastic deformation portion of the indentation process. The methods are derived independently so that future work can be directed at determining the constitutive relationship between stress and strain throughout the development of plastic flow and fracture in a solid material.

Introduction

Molecular dynamics modeling holds great potential as a means of simulating solid materials subjected to nanometer-scale deformation processes. The two most common mechanisms for permanent deformation in solids—plastic flow and fracture—are fundamentally atomistic in nature. It is possible to simulate small-scale processes using molecular dynamics, recapturing the essential atomic behavior of deformation and fracture. Molecular dynamics simulations have the potential to model elastic, plastic, and brittle behavior in a solid. Slip lines for plastic flow and parting lines for fracture are a result of the simulation, rather than an input to it.

In molecular dynamics simulation of solids, each atom (designated by the index i) is modeled as a Newtonian point mass m with position $\mathbf{r}_i$ subject to the equation of motion

$$m\frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{F}_i^{\text{atomic}} + \mathbf{F}_i^{\text{external}} \qquad (1)$$

where $\mathbf{F}_i^{\text{atomic}}$ is the interatomic force on the atom due to all other atoms and $\mathbf{F}_i^{\text{external}}$ is the externally applied force on the atom. A molecular dynamics model with N particles consists essentially of a set of N coupled ordinary differential equations of the form of Equation (1). A Verlet algorithm is typically used to integrate the system for a given set of initial conditions (Gould, and Tobochnik, 1988; Allen and Tildesley, 1987).

The results of a molecular dynamics simulation depend strongly upon the interatomic force model used. Molecular dynamics has been applied most often and most successfully to the study of gases and liquids. In such systems, interatomic forces are primarily due to the primary ionic and covalent bonds, while solid structures interact through the secondary van der Waals bonds (McClintock and Argon, 1966). In metals, there is also an interatomic force due to detachable valence electrons which form a "free electron gas." This electron gas forms the metallic bond, which is a fundamentally quantum mechanical effect responsible for the close-packed crystalline structure of metals. Some aspects of metallic solids, such as macroscopic elastic constants, cannot be modeled accurately by a system of pairwise central forces between atoms (Holian et al., 1991). A noncentral model for interatomic forces in a crystalline lattice was developed by Gibson et al. (1960). A more recent non-pairwise model is the *embedded atom potential* used by Foiles et al. (1986) and Holian et al. (1991). These models attempt to describe the quantum mechanical free electron gas effects as part of the interatomic force in Eq. (1) (Hoover et al., 1990; Hoover et al., 1992; Belak and Stowers, 1990).

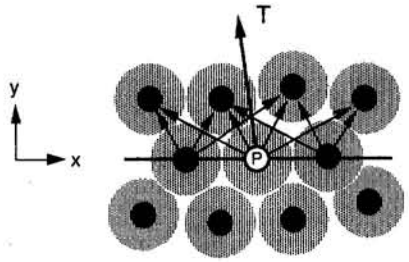

Fig. 1 Two-dimensional sketch of the interatomic forces used to compute the traction vector T at molecule P

One of the current challenges in molecular dynamics is relating simulation results to the macroscopic notions of stress, strain, and the constitutive relation between stress and strain. Evaluation of stress, strain and their relationship is an important check of the quality of the molecular simulation. If the simulation accurately mirrors actual interatomic bonding in a metallic or covalent solid, then one would expect the molecular dynamics simulation of the solid material to exhibit both physically realistic behavior at the *atomic* scale and physically realistic macroscopic relationships between stress and strain. At the atomic scale, realistic material behavior should include stretching or contraction of intermolecular bonds, initiation and propagation of dislocations, and void formation. On a macroscopic scale, realistic material behavior should include elastic deformation, plastic deformation, and possibly fracture, along with naturally occurring transitions among these different stress-strain behaviors. In this paper, independent definitions of stress and strain are proposed by adapting continuum concepts to the dis-

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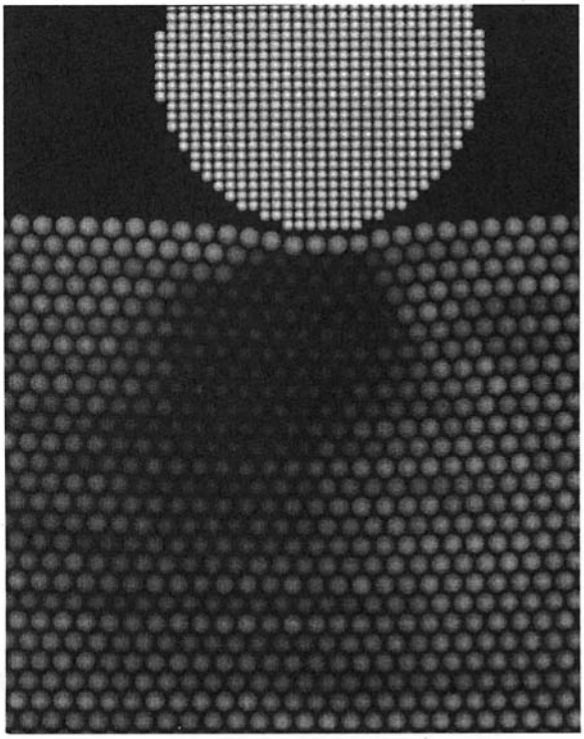

Fig. 2 Map of normalized stress invariant $(\sigma_{xx} + \sigma_{yy})(r^*)^3/\epsilon_o$ in the region beneath the indenter during the elastic phase of indentation. Normalizing constants r^* and ϵ_o are the equilibrium bond length and bond energy, respectively, for the potential function used in this simulation. Values of normalized stress invariant scale with the shade of the atom, with darker shades corresponding to larger compressive stresses.

crete nature of the molecular dynamics model. These definitions can be used in the interpretation and the development of atomic simulations that provide realistic models of solids.

Calculating Stress

Love (1944) has given a definition of stress in particulate systems which is directly applicable to molecular dynamics simulations. A finite segment of a plane is centered on a particular atom. The resultant of all the interatomic forces passing through the plane, divided by the area of the plane is defined as the traction vector, **T**, for the particular atom. Components of the stress tensor are calculated as projections of the traction vector in the coordinate directions. Figure 1 is a two-dimensional sketch of the traction vector **T** at the molecule P. The plane segment centered at P should be small enough to capture the local nature of the interatomic forces, but large enough to give a relatively smooth distribution of the traction vector throughout the body. We have found in the simulations described below that a plane with diameter equal to five times the undeformed interatomic spacing gives stresses that are both locally descriptive and relatively smooth.

Calculating Strain

The strain tensor can be computed using purely geometric information. In continuum mechanics, the strain tensor is defined as

$$\epsilon_{\alpha\beta} = \tfrac{1}{2}(u_{\alpha,\beta} + u_{\beta,\alpha} + u_{\gamma,\alpha}u_{\gamma,\beta}) \qquad (2)$$

where α, β, and γ are coordinate directions, u_α is the Cartesian component of the displacement vector in the α-direction, and a comma denotes differentiation with respect to the coordinate direction indicated by the subscript that follows.

In a molecular dynamics simulation, the displacement vector of each atom is available at each time step. The derivatives in Eq. (2), however, must be approximated using the spatially discrete atomic data. We propose to approximate the derivatives by fitting a linear function to each displacement component at each atom. The discrete displacement data in the neighborhood of a particular atom are used to compute a least squares fit and the slopes of the least squares fit are used to approximate the derivatives. The neighborhood used in the strain calculation should be of the same size as that used in the computation of the traction vector.

Indentation Simulation

We have simulated a two-dimensional indentation of a rectangular workpiece with a rigid, circular indenter. An 8192 processor parallel computer was used, with each processor responsible for one molecule in an initially perfect triangular lattice. The initial atomic velocities were randomly distributed. Interatomic forces were computed using a combination of pairwise central forces derived from a Lennard-Jones potential and noncentral forces derived from the embedded atom potential. A full description of the details of the simulation is given by Scagnetti (1992). The indenter was fixed above the rectangular workpiece for a period of time, allowing the workpiece to come to equilibrium. Next, the indenter moved into the workpiece with a con-

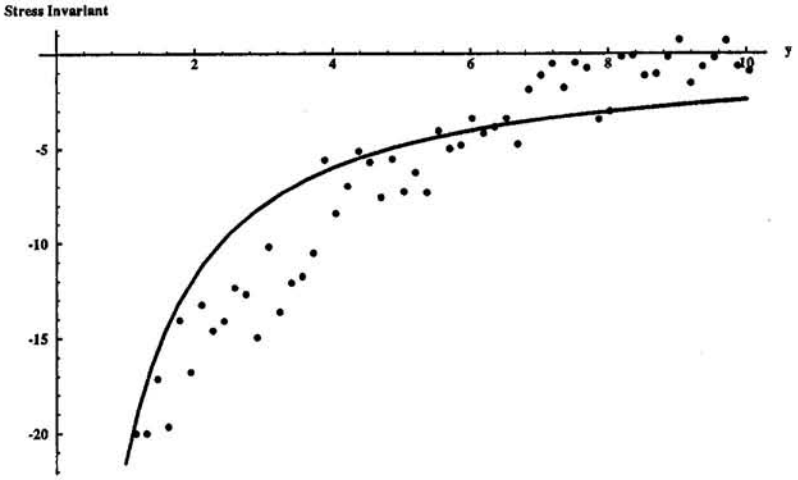

Fig. 3 Plot of normalized stress invariant $(\sigma_{xx} + \sigma_{yy})(r^*)^3/\epsilon_o$, as a function of depth directly beneath the indenter. Solid curve is a continuum Hertzian solution for the same geometry.

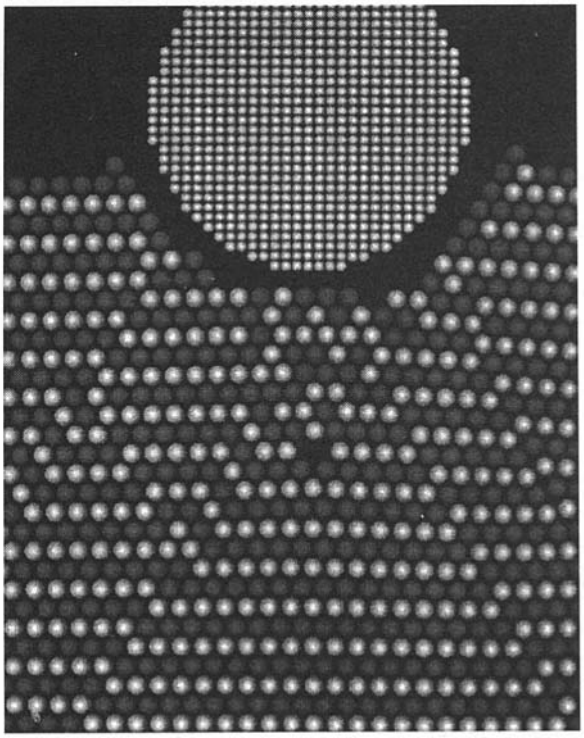

Fig. 4 Plot of molecule positions after indenting to a depth of 10r^*, then retracting the indenter. Atom shading is for visualization only.

stant downward velocity. Finally, the indenter returned to its original position with a constant upward velocity. In the initial phase of indentation, the geometry is very close to that of an elastic Hertzian contact between a cylinder and a semi-infinite half-plane, for which an exact solution exists (Timoshenko and Goodier, 1970).

Results

For the simulations performed, the following observations were made. First, plastic deformation starts to occur as the indenter reaches a depth of about $1.5r^*$, where r^* is the equilibrium spacing between two atoms. Second, the maximum stresses throughout the lattice do not increase after the deformation becomes plastic. Rather, slip lines form, and the stress remains at the maximum elastic value. In this sense, the slip acts to relieve any further stress by propagating dislocations.

At the simulation time shown in Fig. 2, the atomic lattice has deformed in the region beneath the indenter, but there are no discontinuities in the structure of the lattice. If the indenter were removed at this point in the simulation, the lattice would return to its original state. In Fig. 3, the two-dimensional stress invariant ($\sigma_{xx} + \sigma_{yy}$) is plotted as a function of depth directly beneath the indenter. The solid line is the stress invariant predicted by a Hertz analysis. The agreement is very good; better agreement is expected as the number of particles in the simulation is increased, as the speed with which the indenter is moved is reduced, and for initial lattices that more closely resemble a locally isotropic solid. This initial result shows that a molecular dynamics model is capable of producing realistic behavior in the elastic regime, and that our definition of stress can be used to interpret results of a molecular model in a quantitative manner.

Figure 4 shows a section of the lattice at a stage when the indenter has started to move away from the lattice. There is some tendency for the lattice to return to its original configuration ("elastic recovery"), and a stable vacancy or void remains in the lattice. Since voids are an important factor in the process of crack initiation, their natural occurrence in the simulation is a promising indication that atomic simulations can predict the microscopic phenomena that are the ultimate cause of macroscopic material behavior under realistic loading conditions.

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