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Million-Atom Plane-Strain Indentation Studies via Nonequilibrium Molecular Dynamics*

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The long-standing but still-urgent need for a fundamental understanding of plastic flow in precision engineering processing, together with the rapidly-developing promise of inexpensive transputer technology, motivated us to undertake this ongoing basic study of plastic deformation. We are simulating the indentation of metals in plane strain in order to elucidate the size-dependence, rate-dependence, and temperature-dependence of the underlying irreversible constitutive relations.

The simulations considered here cover a range of sizes from fifty to more than one million atoms. We used networked single-processor computers to develop a 64-transputer simulation program for the SPRINT[1] at Livermore. The SPRINT provides the computational speed of a CRAY at 1/1000 the cost.

If the equation of state giving stress as a function of strain were rate-independent, then scale models would accurately predict the behavior of full-scale workpieces. In Figure 1 we show three scale models of a low-temperature indentation simulation. The mean indentor speed, relative to the sound speed, is a few percent. The results shown are for a short-ranged Lennard-Jones potential[2]. The shaded atoms have undergone plastic flow during deformation, as measured by their coordination number. The simulations shown here, ranging up to 12,800 atoms, were carried out on the Euler work station at Keio University. All of our simulations use a modified Stoermer version of Nosé-Hoover nonequilibrium molecular dynamics[3]. The dynamics is time-reversible, highly stable, and well-suited to nonequilibrium simulations. The kinetic temperature is maintained through a time-reversible friction coefficient ζ:

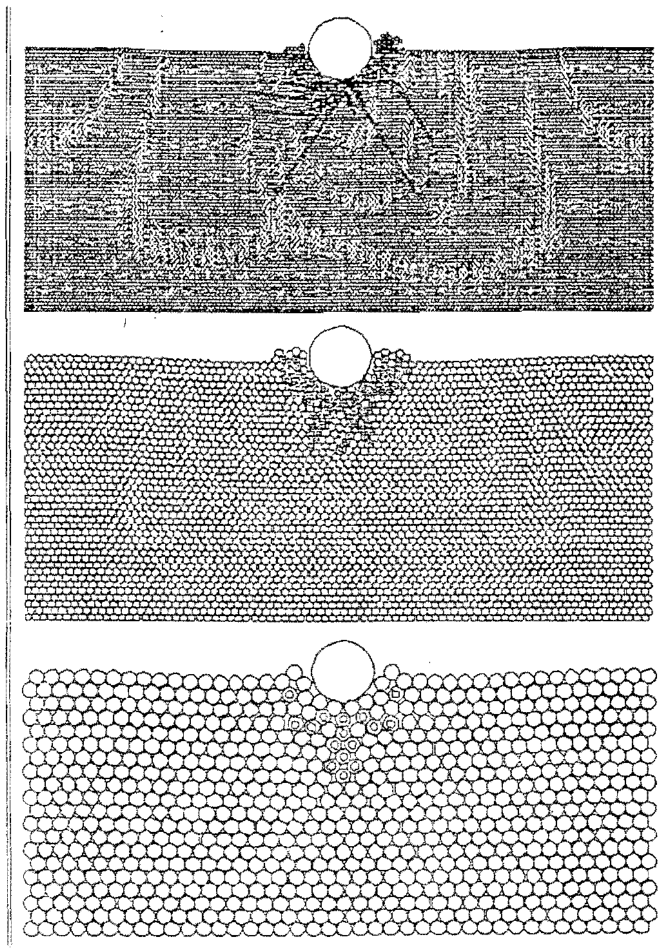
$$r(t+dt) - 2r(t) + r(t-dt) = [F(r(t))(dt)^2/m] - \zeta(t)[r(t+dt) - r(t-dt)](dt)/2 ;$$
$$\zeta(t+dt) - \zeta(t) = [(K(t+(1/2)dt) - K_0)/K_0](dt)/\tau^2 .$$

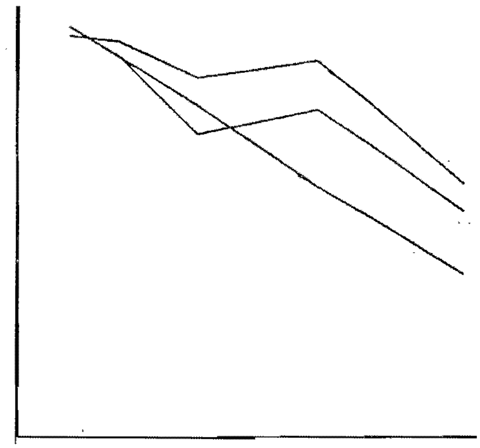
The centered kinetic energy, $K(t+(1/2)dt)$, is calculated from the coordinates $r(t+dt)$ and $r(t)$. K_0 is the equipartition, long-time-averaged value of the kinetic energy.

We have already verified that our results are insensitive to the type of interaction between indentor and surface atoms, and to the time scale τ of the Nose-Hoover thermostat. We are presently investigating the size and rate dependences which will need to be explicitly included in continuum models of the indentation process or in related models describing surface cutting and polishing.

As the simulation scale is increased the results must approach the predictions of continuum mechanics. Up to 12,800 atoms the specific work of deformation varies in a systematic way with the inverse problem size. See Figure 2. Results are included in that Figure for a two-fold reduction in indentor rate as well as for a smoothly-truncated Hooke's-Law potential having the same zero-pressure density and sound velocities as the Lennard-Jones potential.

The simulation on the SPRINT uses a linked list to locate atoms within processors, transferring atomic coordinates between processors at the end of each Stoermer time step. Atoms within each processor are further divided into cells, with each cell holding just a few atoms. The transfer operations take a negligible fraction of the clock time per time step, measured at 36 seconds for 1,000,000 particles with 64 processors. It is clear that *billion-particle* simulations require no more than the cost of a CRAY computer, invested in a 65,536-transputer version of the SPRINT.





The energy density(vertical) as a function of the inverse system size (horizontal) for indentation simulations with 50, 200, 800, 3200, and 12800 atoms. The upper two curves show the effect of a twofold reduction in the indentation rate. The higher curve corresponds to an average speed of $0.50(\varepsilon/m)^{1/2}$ and the middle curve to an average speed of $0.25(\varepsilon/m)^{1/2}$. The nearly straight curve corresponds to Hooke's-Law indentation at the higher of the two rates.

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3. For recent references see B. L. Holian, G. Ciccotti, W. G. Hoover, B. Moran, and H. A. Posch, Phys. Rev. **A** 39, 5414 (1989).