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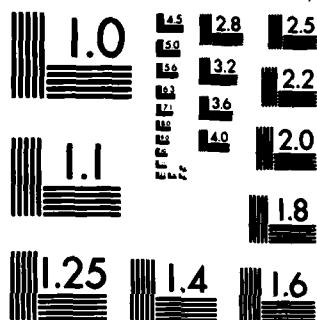
CONFORMATIONAL AND MECHANICAL PROPERTIES AT HIGH STRAIN 1/1
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Plastic Flow
PlasticityPowder Compaction
Fracture Properties

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

We have developed several powerful means of studying steady flows far
from equilibrium. ^{not developed} Gauss' Principle (minimizing the forces of constraint) was
found to be useful for most problems, but leads to (small, 10%) errors when
applied to heat flow simulations.

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20. ABSTRACT CONTINUED:

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We have discovered ^{were} corresponding-states relations for the rate-dependent viscosity and flux-dependent heat conductivity which are useful in making macroscopic constitutive-equation estimates.

Additional keywords:
mechanical properties; plastic flow; plasticity;
power compaction; fracture properties; Army research.

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Final Report to
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Research Triangle Park, North Carolina

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Scientific Personnel Supported: William G. Hoover, Principal Investigator
J. Andrew Combs
Anthony J. C. Ladd
Carlo Massobrio

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Submitted by:

A handwritten signature in dark ink, appearing to read "W. G. Hoover".
William G. Hoover

Problem Studied

As stated in our proposal of 2 April 1981, "Conformational and Mechanical Properties at High Strain Rates," fundamental knowledge of high-speed deformation is very limited. We have provided new insights both on the microscopic atomistic level and at the macroscopic level of constitutive modelling.

During our 42-month study we have analyzed the plastic flow of solids (1, 2, 3) reviewed and developed new simulation methods for studying mass, momentum, and energy flows (4, 5, 6, 7, 8, 9). We have considered the macroscopic aspects of plasticity, fracture, and powder compaction (10, 11, 12). We have begun an extension of these ideas to molecular systems (13) and have considered the technical aspects of some simple problems in elasticity (14, 15). We have most recently studied heat flow simulation in fluids and solids (16).

Summary of Results

We have developed several powerful means of studying steady flows far from equilibrium. Gauss' Principle (minimizing the forces of constraint) was found to be useful for most problems, but leads to (small, 10%) errors when applied to heat flow simulations.

We have discovered corresponding-states relations for the rate-dependent viscosity and flux-dependent heat conductivity which are useful in making macroscopic constitutive-equation estimates.

We have stimulated considerable interest in this area through a series of review articles and through participation in and organization of several international meetings and schools* covering these areas.

*National Bureau of Standards at Boulder (1982)
Orsay CECAM Workshops at Orsay (1983-5)
Euratom Course at Ispra (1984)
Enrico Fermi School of Physics at Varenna (1985)

Related Publications

1. Hoover, W. G., A. J. C. Ladd, and B. Moran. High-Strain-Rate Plastic Flow Studied via Nonequilibrium Molecular Dynamics. *Physical Review Letters* 48:1818-1820.
2. Ladd, A. J. C., and W. G. Hoover. Energy and entropy of interacting dislocations. *Physical Review B* 26:5469-5479.
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4. Hoover, W. G. Atomistic Nonequilibrium Computer Simulations. *Physica* 118A:111-122.
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7. Hoover, W. G., A. J. C. Ladd, and V. N. Hoover. Historical Development and Recent Applications of Molecular Dynamics Simulation, p. 29-46. In J. M. Haile and G. A. Mansoori (Eds.), Molecular-Based Study of Fluids, American Chemical Society, Washington, D.C.
8. Hoover, W. G. Computer simulation of many-body dynamics. *Physics Today*, January:44-50.
9. Hoover, W. G. Canonical Dynamics. Equilibrium Phase-Space Distributions. *Physical Review A*.
10. Hoover, W. G. Simulation of Brittle Fracture Via Molecular Dynamics. Ispra Courses Proceedings Series, Ispra, Italy. 1984.
11. Hoover, W. G. Flow and Plasticity Via Nonequilibrium Molecular Dynamics. Ispra Courses Proceedings Series, Ispra, Italy. 1984.
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16. Hoover, W. G., B. Moran, and J. M. Haile. Homogeneous Periodic Heat Flow via Nonequilibrium Molecular Dynamics. *Journal of Statistical Physics* 37:109-121.

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