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COMPUTER SIMULATION
IN
PHYSICAL METALLURGY

Lectures delivered at the ISPRA-Course held at Ispra,
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DYNAMIC COMPACTION OF POWDERS

WILLIAM G. HOOVER

1. INTRODUCTION

Powder metallurgy and explosive forming are both well-established technologies. With powder metallurgy, relatively complex parts, requiring little machining, can be made by casting or by static compression of powdered metals or ceramics. The voids and irregularities in the powders can be reduced by exposure to high-temperature, "sintering", to strengthen the finished product. With explosive forming, large, relatively simple shapes can be made. Costly large-scale static presses can be replaced by transient pressure waves created by detonating high explosives. The powder-metallurgy and explosive-forming methods, were first combined, in dynamic compaction, about 25 years ago.[1,2] The purpose was to make parts from nonequilibrium powders which were either hard to compact or which might lose their unique properties in the high-temperature sintering operation. Just as in ordinary explosive forming, dynamic compaction has the advantage of lighter-weight equipment. The main disadvantages are, first, the noise and vibration associated with high explosives and, second, the material inhomogeneities produced by dynamic loading.

There are many methods for making nonequilibrium powdered materials. The distribution of powder particle shapes, sizes, grain structure, and hardness can be varied widely. Most methods use high-speed cooling. The particles

G. Jacucci (ed.), Computer Simulation in Physical Metallurgy, 69–85.

themselves can be made from bulk materials using mechanical, inertial, electrical, or thermal separation methods. Because the time required to cool a conducting object varies as the square of its size, separated powder particles can be cooled much more rapidly than bulk matter. Thus the most interesting nonequilibrium materials are available in the form of powders. Such powders can be consolidated into technologically useful bulk materials either by static presses or by dynamic compaction. Dynamic processing enhances locked-in elastic strains and lattice defects, often resulting in a stronger material. Because the dynamic high-pressure state is transient, lasting only nanoseconds or microseconds, the whole compacting process can be completed before thermodynamically immiscible components of the powder particles have time to separate. Thus dynamic compaction can lead to nonequilibrium materials with unique mechanical, electromagnetic, or chemical properties.

The dynamic methods involve sufficiently complicated and inhomogeneous material behavior and geometrical wave-propagation effects, that numerical simulation is a relatively inexpensive and attractive way to predict the effects of changing experimental parameters. The dynamical process of powder compaction, using explosively-driven shock waves, is well-suited to numerical simulation.

On the most fundamental, atomic, level, nonequilibrium high-strain-rate simulations[3] should prove useful in understanding the compaction process. Presently, computer simulations are restricted to a few thousand particles. Simulations involving more particles but with much less realistic interactions can be carried out with bubbles. Figure 1 shows two stages in a "bubble-raft" simulation of the sintering process. In the movie version of this simulation, nucleation and motion of dislocations are readily followed.[4]

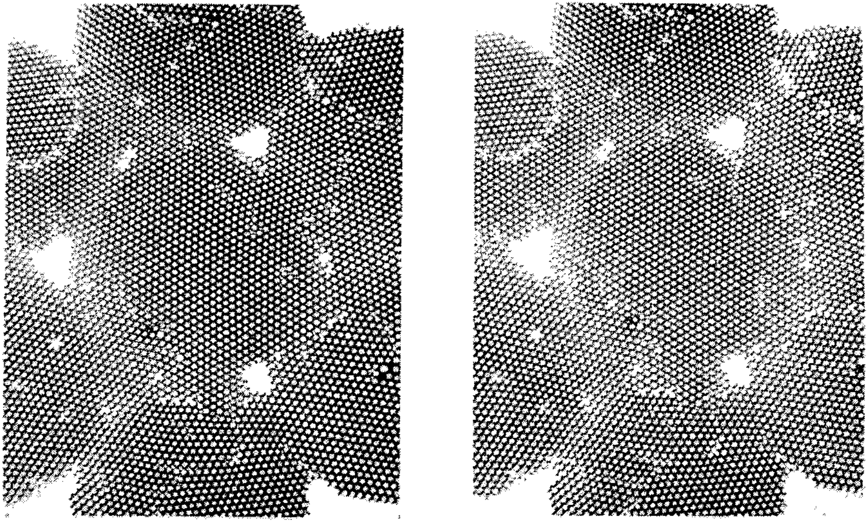


Figure 1. Bubble-raft model of copper-powder sintering from reference 4.

On the macroscopic scale, computer solution of the partial differential equations of motion can be used to provide a realistic model of compaction. To do this, equations of state for metals, powders, and high explosives all must be included. Here I describe some of the simulation work carried out by Mark Wilkins, at the Lawrence Livermore National Laboratory, modeling dynamic compaction. His finite-difference simulations of dynamic compaction were carried out in parallel with corresponding laboratory experiments. He will present a comprehensive report at the San Antonio (Texas) High-Energy-Rate Fabrication meeting next month.[5]

2. NONEQUILIBRIUM POWDERS

Whether a state of matter is "equilibrium" or "nonequilibrium" depends upon the timescale of observation. From the standpoint of a nuclear physicist, the stable form of matter is iron. From the standpoint of thermodynamic stability, graphite is stable under normal conditions while diamond is not. From the standpoint of a physicist at dinner, oil-and-vinegar salad dressing is sufficiently stable for prompt use. Under ordinary conditions, diamond has a reasonable lifetime, much longer than that of an oil-and-vinegar emulsion. Diamond powder can be produced by compressing graphite. Because the economic value of diamonds increases in a nonlinear way with size, it is commercially feasible to compact diamond powder into macroscopic pieces useful for machinery, and possibly, for jewelry.

Diamond is only one example of the many metastable forms of matter with desirable properties. Mechanical and electrical properties can often be improved by using nonequilibrium compositions. For instance, amorphous metals, made by rapid quenching of a melt on the surface of a cold substrate, can have much higher mechanical strengths than do their stable parent ingredients. This is because the principal mechanism for plastic flow in metals, dislocation motion, is not available to a material lacking crystalline order. Flow can also be inhibited by an admixture of atoms of different size.

For a list of more than 80 materials, metals, alloys, ceramics, and composites, all of which have been compacted dynamically, see page 55 of reference 2.

3. SHOCK AND DETONATION WAVES

Typical solid yield strengths can be estimated by noting that Mount Everest must exert a pressure of a few kilobars on the supporting earth beneath. Failure of the earth to flow, in the presence of this stress, suggests that solid yield strengths are also a few kilobars. Static apparatus designed to compact powders must, accordingly, be capable of exerting such pressures over areas of several square centimeters. The need for a supporting rigid structure can be eliminated if the high pressure is produced within a transient pressure wave that need not be supported by material boundaries. Such waves can be generated by using high explosives.

The energy-density of typical explosives, relative to their reaction products, can accelerate metals to velocities of a few kilometers per second. This speed corresponds to an energy density of hundreds of kilobars, fully adequate to provide the pressures necessary for the irreversible deformation and compaction of solids, even diamond.

Steady shock or detonation waves convert one equilibrium state of matter into another through an adiabatic process conserving mass, momentum, and energy. In the case of detonation waves, which drive shockwaves, the explosive's potential energy is divided between external work done and heat of its reaction products.

In a monatomic fluid a typical shockwave has a thickness on the order of an atomic diameter.[6] Figure 2 shows the variation in density, pressure, energy, and temperature in such a fluid-phase shockwave. The distance scale is measured in atomic diameters. The curves were calculated using the Lennard-Jones equation of state and state-dependent transport coefficients in the Navier-Stokes equations. The circles come from molecular dynamics simulations.[6] The strength of the shockwave in these calculations carried

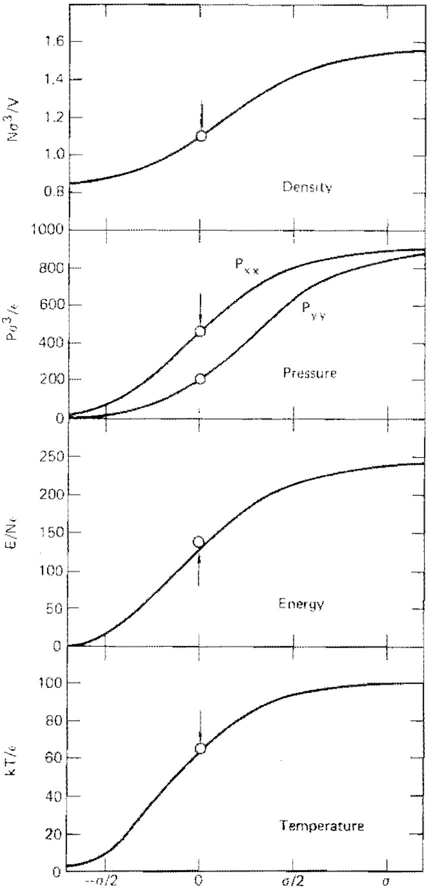


Figure 2. Dense-fluid shockwave.

triple-point argon to about 400 kilobars, with a final temperature of about one electron volt.

Because shockwaves move somewhat more rapidly than sound, the typical time for conversion from initial to final state, in a monatomic fluid, is only about a picosecond.

If relaxation processes must occur from excited states (vibrational or electronic, for example), then the shock process takes more time. In solids, deformation involves cooperative nonlocalized motion. This lack of localization serves to spread out the macroscopic shock zone. Nevertheless the shock process can be completed before structural or chemical changes occur. Typical powders are made up of micron-sized particles, a few hundred atoms in diameter. A typical shockwave travels at speeds of order one kilometer per second. Such a micron-sized particle will therefore be traversed in about one nanosecond. Thus the deformation rates near voids, at which the gaps between powder grains are filled in by deforming material, must be 10 gigahertz or more. Friction and stress-wave reflections at these gaps can cause intense local heating, melting, and jet formation. On the scale of individual grains, the compaction process is violent and inhomogeneous.

The time required for thermal equilibration of a micron-sized metal particle is about a nanosecond (assuming a thermal diffusivity of about one square centimeter per second). Thus localized melting, vaporization, and light emission can be expected to occur during shock compaction.

Computer simulations of homogeneous high-strain-rate deformation in solids are consistent with the limited information available from plastic wave-shape experiments. The "nonequilibrium molecular dynamics" simulations are carried out with shearing boundary conditions, changing with time. Typically, a few hundred atoms are used and the deformation proceeds to a total strain of order 100. As the system is sheared, plastic work is done. To avoid the irreversible heating associated with this work, the equations of motion are additionally constrained to preserve the temperature or the energy unchanged. Thus nonequilibrium simulations of high-strain-rate flow can be carried out in the desired steady state.[7]

Figure 3 is a corresponding-states description of the dependence of yield strength on strain rate. The figure includes both atomistic simulation data

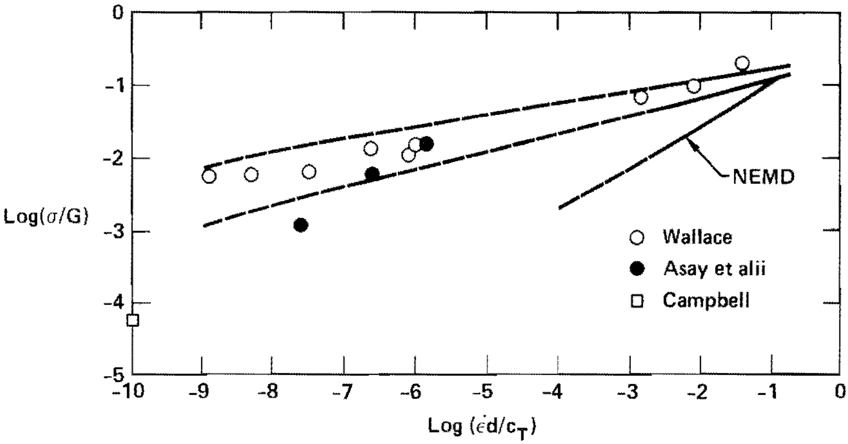


Figure 3. Solid-phase shear stress σ as a function of strain rate $\dot{\varepsilon}$.

(solid lines on the righthand side of the figure) and experimentally-based estimates (points on the lefthand side) for the yield strength as a function of strain rate. G is the shear modulus, d is the interparticle spacing, and c is the transverse sound speed. The maximum strain rate shown in the figure exceeds a terahertz and corresponds to neighboring atoms shearing past one another at approximately the velocity of sound.

Together, the simulation results, and the experimental evidence[1], provide ample reason to believe that the yield strength during dynamic shear deformation substantially exceeds its static value. For a yield strength of 10 kilobars and a total plastic strain of unity, the work of deformation would provide a temperature increase of several hundred kelvins. Much higher temperatures would be expected near the surfaces of non-spherical powders, or for powders with higher yield strengths.

4. LAGRANGIAN SIMULATIONS[8]

In a typical "finite-difference" (as opposed to differential) computer program, a structure is divided up into comoving "Lagrangian zones." These zones are just line segments in one-dimensional simulations. Zones are usually triangular or four-sided in two dimensions, and six-sided polyhedral "bricks" in three dimensions.

These continuum simulations are more complicated than atomistic ones because each zone has <u>many</u> properties (the stress and strain-rate tensors, for instance) which must be followed as functions of time, not just location and velocity. Just as in the atomistic case[9], simulations involving thousands of zones are possible. For a typical calculational grid, see figure 4. In the figure each rectangular zone represents a ring of material (powdered metal, confining plastic tube, or high explosive, from inner radius to outer

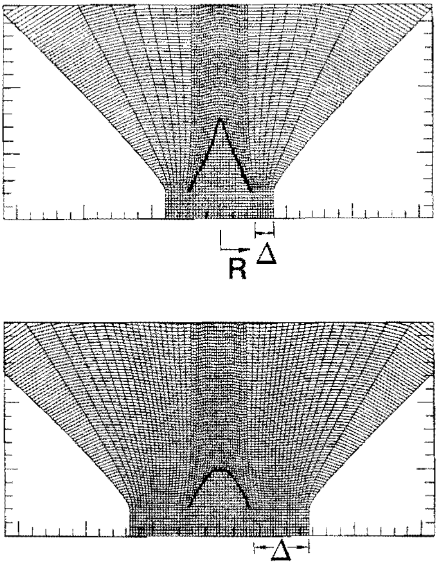


Figure 4. Explosive compaction. The maximum radius shown is 15 centimeters.

boundary) in a geometry with cylindrical symmetry. The cylindrical axis is vertical. The region originally filled with explosive is indicated by Δ. At the instant shown in the picture the detonation wave in the explosive has progressed from the top surface of the cylinder nearly to the base. The fanshaped region is made up of expanding Lagrangian zones filled with hot product gases from the detonating explosive. The motion of each of the materials shown (explosive, plastic, and powdered metal) obeys finite-difference approximations to the continuum equation of motion, $\rho\dot{u} = \nabla\cdot\sigma$. Stress σ and strain ε in each zone are approximated in terms of boundary "node" displacements, leading to ordinary differential equations for the motion of these nodes. How are the finite-difference equations converted into ordinary differential equations?

As a simple example, consider a meter stick divided into 100 1-cm zones by 101 equally spaced nodes. Now consider longitudinal deformations. In the elastic regime the longitudinal stress in each zone would be given by Young's modulus E times the strain, $\varepsilon_{xx} = (V - V_o)/V_o$. By considering the stress levels in the two zones adjacent to each node, the accelerations $\ddot{x}_j$ can be calculated. The differential-difference equation of motion for a typical node has the form

$$m\ddot{x}_J = E(x_{J+1}-2x_J+x_{J-1})/d \quad , \qquad (1)$$

where m = ρd is the mass of a zone and d is the unstrained zone length. If we fix the two ends of the meter stick, ($x_1 = 0$, $x_{101} = 100$) this problem can be solved analytically. With the nodal displacements given by $x_J = A \exp(i\omega t - ikx_J^0)$, the equations of motion lead to the eigenvalue solution for the vibration frequency ω, as a function of the wave-vector k:

$$\omega^2 = (E/\rho d^2)\ (2-2\cos kd) \quad . \qquad (2)$$

This solution corresponds to the exact continuum solution, $\omega^2 = (E/\rho)k^2$, in the limit that d vanishes. For nonzero d the error is of order d^2. An explicit finite-difference solution of equation (1) would typically be carried out by approximating the second-order time derivative,

$$\ddot{x}_J(t) \doteq [x_J(t+dt) - 2x_J(t) + x_J(t-dt)]/(dt)^2 \quad . \qquad (3)$$

Here again the errors in the finite-difference approach are second order, of order $(dt)^2$.

The set of 99 difference equations resulting from combining the spatial discretization in (1) with the temporal discretization in (3) can <u>still</u> be solved by the plane-wave solution appropriate to (1), but the solution is unstable, and diverges exponentially in time, unless dt is sufficiently small. The numerical instability can be analyzed by examining the high-frequency motion in which adjacent nodes move in opposite directions, kd = π. The quadratic equation for exp($i\omega t$) produces unstable solutions unless dt is less than the time required for sound to cross the zone width d, dt $<$ d/c, where the sound speed c is $(E/\rho)^{1/2}$. This condition on dt, called the Courant condition, is necessary for stability. The analysis is obviously more complicated by geometrical and constitutive nonlinearities, but the principle applies to any explicit finite-difference solution of the equations of motion.

In applying the numerical explicit finite-diffence approach to powder compaction, there are two additional complications. Both the equation of state of a porous (powder) material and the equation of state of the explosive driving the material must be specified. For powders, the simple interpolative equation of state

$$(V_o/V) = (1 + AP) / (1 + BP) \quad , \qquad (4)$$

where A and B are chosen to match the powder's initial compressibility and density, is sufficiently accurate for many purposes. An accurate version would have to include more parameters as well as an explicit dependence on energy and the size and surface finish of the powdered material.

For high explosives the equation of state is energy-dependent and time-dependent. The detonation energy (taken from experiment) in each zone is released at the time and with a rate consistent with the (experimental) detonation speed.

In dynamic compaction both the magnitude and duration of the stress are important. Because dynamic pressure waves move at approximately sonic velocities, the relative values of the sound speeds in the explosive and in the material being compacted are crucial to determining the stress history followed by the material. Figure 5 shows the difference between a fast and slow explosive (relative to the sound velocity in the steel) compressing a stack of four steel plates.

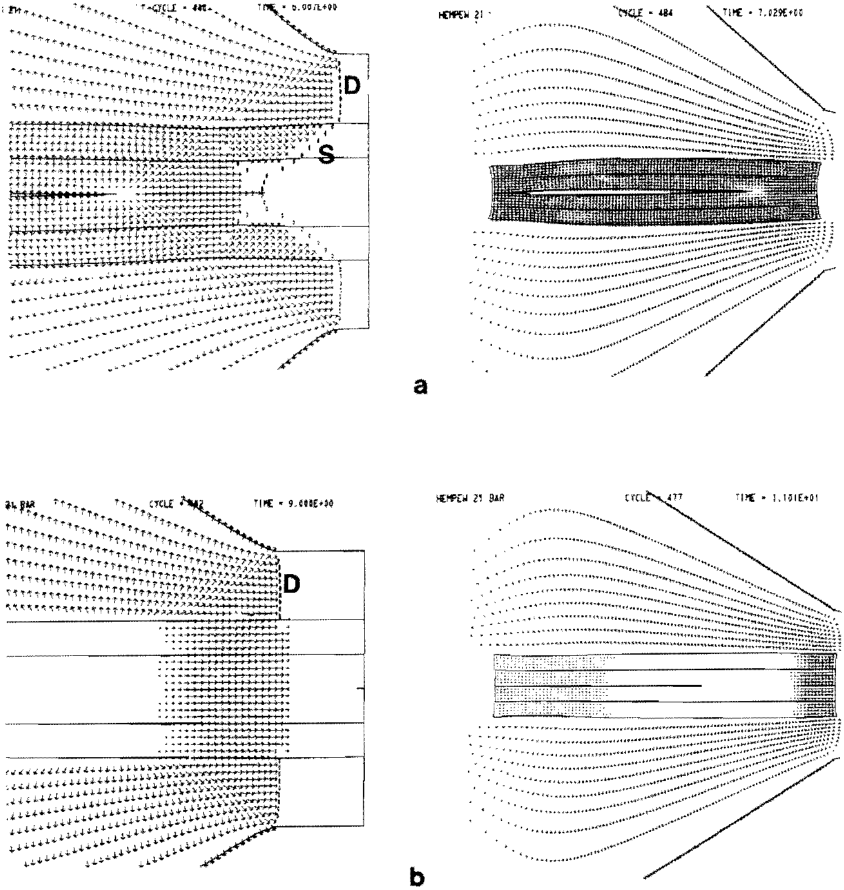
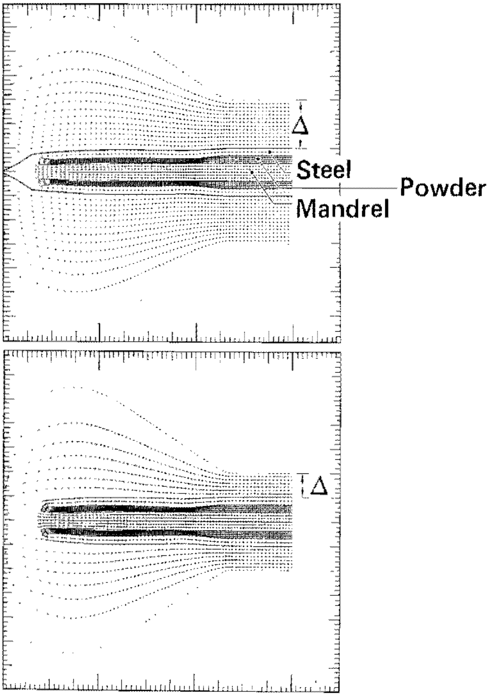


Figure 5. Fast (top) and slow (bottom) explosive compression processes.

There are explosive charges both above and below the stack of steel plates. In the fast-explosive case a strong shockwave is formed. At the horizontal centerline the high pressure generated is sufficient to force the plates apart, releasing the stored compression energy. The compression occurs too rapidly. This undesirable behavior can be avoided by using a slower explosive. In that case (baseof figure) the pressure waves in the steel can outrun the detonation wave (D) in the explosive, resulting in permanent plastic deformation.

Because a considerable part of the energy lost by compression waves in compressing and compacting powders, typically at only half normal density, offsets the gain from cylindrical stress convergence, it is possible to achieve a fairly uniform stress level. Computer simulations are particularly useful in studying the variation of results with changing geometrical features. If too little explosive is used, losses predominate and powder near the center of the cylinder is not compacted. If too much is used, the central region can be melted or vaporized by stress convergence. A method for moderating excessive compressive stresses (which can cause melting) or tensile stresses (which can cause cracking) is to place a massive "mandrel" along the cylinder axis. This geometry is shown in figure 6 for two different thicknesses (Δ) of explosive.

The dynamical properties of the mandrel influence the quality of the compacted powder. The effect of an aluminum core within a steel mandrel is illustrated in figure 7, in which copper powder was compressed. In the upper photograph a pure steel mandrel was used. In the lower photograph the steel contained a central aluminum bar. The softer aluminum cushioned the compacting powder better the compacting powder better than did the steel, which exhibits the multiple fractures characteristic of excessively-strong rarefaction waves. The calculations shown in the figures all correspond to real laboratory experiments.



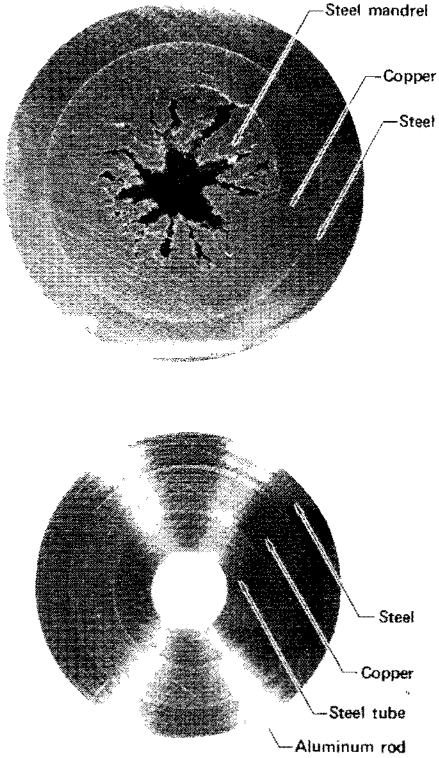


Figure 6. Cylindrical powder compaction with central mandrel. Two explosive thicknesses (Δ).

Figure 7. Cylindrical compaction of copper powder. Steel mandrel with and without aluminum filler.

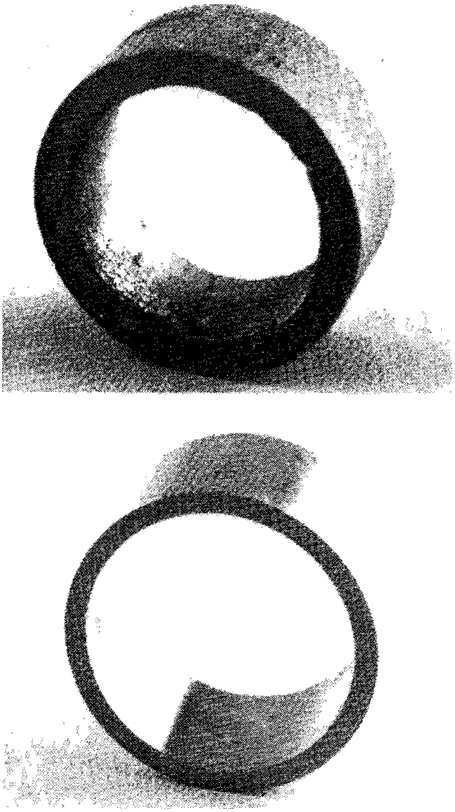


Figure 8. Aluminum nitride and metallic glass cylinder.

The sections of aluminum nitride (top) and metallic glass (bottom) cylinders shown in figure 8 were both made using aluminum mandrels. Because the equation of state of powders is complicated by the effects of grain size, hardness, shape, and surface oxidation, and is not simply related to the equation of state of the parent materials, series of simulations must be carried out to make the parameters of the equation-of-state models fit experimental results. Once this fitting procedure has been accomplished, the resulting model is capable of predicting the results of further experiments.

6. OUTLOOK

The potential importance of dynamic compaction, coupled with the sophistication required for effective modeling make dynamic compaction an exciting area of physics right now. In particular, microscopic modeling of surface-surface interactions, and mesoscopic modeling of sintering, deformation, and cold welding should have useful impact on the macroscopic models required to help design physics experiments and refine commercial powder processes.

7. PROBLEMS

A. Calculate the minimum radial strain required to change a disk to a hexagon at fixed density. If only the outer half of the disk deforms, what is the minimum strain required?

B. Show that the time required for a grain to reach uniform temperature varies as the two-thirds power of its volume. Assume that heat flow follows Fourier's law $\dot{T} = D\nabla^2 T$, where the thermal diffusivity D is constant.

C. Show that the finite-difference solution for the vibrations of a meter stick fails to converge if the Courant condition $dt < d/c$ is violated.

ACKNOWLEDGMENT

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