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A METHOD OF DETERMINING POINTS ON THE PRINCIPAL ISENTROPES OF MOLECULAR LIQUIDS

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ABSTRACT

We have examined the feasibility of using a large-diameter, projectile-target impact to carry out one-dimensional, isentropic compression experiments on molecular fluids. By employing a three-layered target geometry, with a thin foam driver layer and a thick, high-impedance anvil layer, liquid H_2O can be compressed to a state within 0.1% of its principal isentrope at pressures up to about 30 GPa. The pressure and density of the state achieved can be determined from electromagnetic particle velocity gauges imbedded on the interfaces bounding the sample.

INTRODUCTION

Because of the relative simplicity of shock wave experimental techniques, most high pressure data obtained for dynamically compressed materials have been Hugoniot data. However, there are many problems--particularly involving low impedance materials such as molecular fluids--for which knowledge of the principal isentrope would be of great value. Several methods have been conceived for the production of large isentropic compressions in one dimension,[1-5] none of which seem to be directly amenable to measurement. The most likely configuration for an experimental attempt is a simplified version of the symmetric impact experiment proposed by Lyzenga[4] and Lyzenga and Ahrens[5] (Fig. 1).

This experiment involves the use of several layers with large shock-impedance contrast arranged in a way such that the sample layer is compressed by a series of small shocks, as opposed to a single large shock wave as in a conventional Hugoniot experiment. This idea is based on the principle that a compression will be isentropic in the limit of small shocks. Because it has been found empirically that in such a configuration, the net entropy gain is controlled by the first shock wave,[4,5] a low density foam layer (Fig. 1, Material I) is used to break up the initial shock wave into small shocks before it enters the sample layer (Material II). These two layers then reverberate together up to some peak pressure dictated by the high impedance of the flyer and anvil layers (Material III in Fig. 1, but not necessarily the same material).

Another attractive property of using foam for the first layer is that it can be chosen so that above its crush-up pressure it is a good impedance match to the sample layer, so rarefactions and re-compressions, which increase the final entropy, are avoided.

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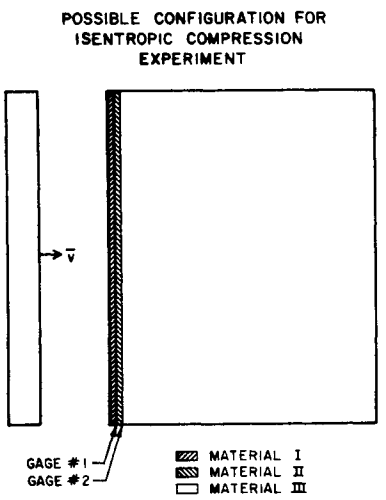

Fig. 1. Three-layer target for producing isentropic compressions is impacted by flyer plate at velocity $\bar{v}$. Shock impedance increases from material I to III.

However, it takes about ten shock wave transits to reverberate up to peak pressure. As a result, the flyer and anvil must be about twenty times as thick as the other layers combined in order to prevent rarefactions from the free surfaces from entering the sample layer. This constraint, along with the constraints imposed by edge effects, requires us to consider a sample layer with a thickness on the order of only a few millimeters for a realistic laboratory experiment.

COMPUTER SIMULATIONS

Several variations of this three-layered target geometry were tested using a one-dimensional finite difference code.[6] A simplified equation of state (EOS) was assumed for H_2O, with a linear u_s-u_p relationship, where c_o = 2.335 mm/μsec and s = 1.359 are taken from a fit to published data.[7,8] For the foam layer, we used parameters approximating a polyurethane reference EOS,[9-11] with an initial distension of 10.0, a foam yield stress of 0.02 GPa and a crush-up stress of 0.2 GPa. The important aspects of the simulation were insensitive to variation of the foam parameters.

A greater effort was made to use accurate parameters for the anvil layer, because these dictate the final sample pressure. A high impedance insulator is necessary; high impedance to achieve high peak pressures, and insulating to allow use of electromagnetic gauges. We used parameters for polycrystalline Al_2O_3, which has been studied in detail up to 16 GPa.[12] The constitutive equation for this layer includes an elastic limit and strain rate dependence.

RESULTS AND DISCUSSION

Several simulations were run in the configuration shown in Fig. 1, varying parameters such as velocity, layer thickness, and foam constitutive equation. In the case shown in Fig. 2, the foam layer was 0.5mm, the H_2O layer was 1.0mm and the Al_2O_3 layer was 40mm thick. The "infinite impedance" flyer velocity was 0.75mm/μsec. This is roughly (but not exactly) equivalent to an Al_2O_3 flyer with a velocity of 1.50mm/μsec.

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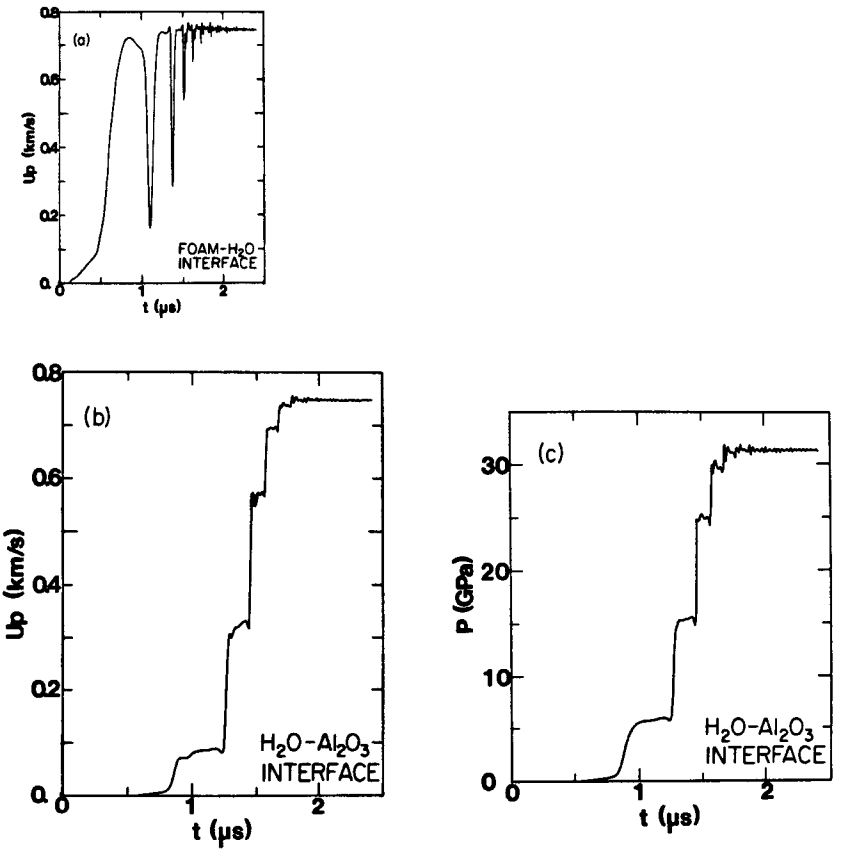

Fig. 2. Particle velocity (Up) and pressure (P) histories calculated by finite difference code for a simulated impact on a three-layer target. (a) $u_p(t)$ at left boundary of sample layer. (b) $u_p(t)$ at right boundary of sample layer. (c) P(t) at right hand boundary of sample layer.

The particle velocity histories at the H_2O layer interfaces are shown in Figs. 2a and 2b, and the pressure history at the H_2O-Al_2O_3 interface is shown in Fig. 2c. These illustrate the effect of the foam in breaking up the first shock wave. The first disturbance is effectively a shallow ramp wave up to about 1 GPa. After a few reflections, the ramp steepens into a shock, but by then the shock waves are not as dissipative, or entropy-producing. By 2.0 μsec, the right-hand interface of the H_2O has reached 31.4 GPa, and a density of 2.18 g/cm^3. The calculated pressure on the isentrope of H_2O at this density is 31.39 GPa, while the Hugoniot pressure is 42.76 GPa. Thus the non-isentropicity in this experiment is clearly negligible. The difference in pressure across the H_2O layer after 2 μsec averages about 0.1 GPa, well less than 1% of the total

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pressure. For realistic measurement precisions, effects of non-isentropicity and non-uniformity are therefore not important.

The density of the H_2O layer can be determined by integrating the difference of the particle velocities of its interfaces over time, by the equation

$$\eta(\tau) = \left(1 - \frac{\rho_o}{\rho}\right) = \frac{1}{x_o} \int_o^T (u_{p1}(t) - u_{p2}(t))dt \qquad (1)$$

where $u_{p1}(t)$ and $u_{p2}(t)$ are the velocities of the left- and right-hand interfaces, respectively, and x_o is the initial thickness of the layer. The particle velocities at these interfaces can be measured by electromagnetic gauges,[13] which have an experimental uncertainty of about 1%.[14] This uncertainty combined with a 1% oscilloscope uncertainty leads to a net uncertainty of about 2% in the final density measurement. At times prior to 2 μsec in our simulation example, the density determined in this manner is meaningless, because of the non-uniformity of the layer (a shock wave being in transit); however, it may be possible to determine the intermediate states at the moment the shock wave is reflecting from one of the boundaries.

There are several possible methods of determining the pressure, the simplest being an impedance match solution for the final (peak) state. This method would not give pressures of the intermediate states, however, and is limited by knowledge of the outer-layer parameters. If the anvil is a well-studied material, as the polycrystalline Al_2O_3 is below 16 GPa, the particle velocity at the left boundary of the anvil can be used with the anvil constitutive equation to obtain a stress history at that boundary, providing no rarefaction has arrived from the anvil free surface. If the anvil material has a strain-rate dependence, the velocity of the interface can be used as a boundary condition along with the material parameters in the one-dimensional code to obtain the stress. If there is no rate dependence, the Riemann integral can be inverted to obtain $P(u_p)$.[15] In cases where the material properties are not well known, it may be necessary to use an inclined electromagnetic gauge,[16] or Manganin stress gauge. By one or a combination of these it may be possible to determine the peak pressure to an uncertainty of about 2%.

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