A MOLECULAR DYNAMIC STUDY OF THE THERMODYNAMIC BEHAVIOR OF A THIN FILM UNDERGOING HYPERVELOCITY PENETRATION

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Introduction: A renewed interest in the study of hypervelocity penetration events has been sparked by concerns about the survivability of a permanent Space Station in Low Earth Orbit. Empirical evidence concerning orbital debris and Interplanetary Dust Particles has been gathered by LDEF, Solar Max, and experiments being flown on the STS. A correct understanding of this data requires an understanding of the properties of hypervelocity impacts. Theoretical studies of hypervelocity events have generally employed the hydrodynamic equations of motion and attempted to solve these equations numerically. Various schemes have been developed and many software packages written that use a Eulerian, Lagrangian or a hybrid mesh to numerically solve the hydrodynamic equations of motion. The use of continuum models requires a knowledge of the Equation of State for the materials undergoing the hypervelocity impact. One alternative to the use of hydrodynamic modeling is to employ a Molecular Dynamic (MD) simulation of the hypervelocity events as used by Holian. The only apriori knowledge required is the intermolecular potential governing the behavior of the molecules or atoms. The relationship between MD and hydrodynamics has been established, but is beyond the scope of this paper.

Molecular Dynamics: Here a thin film was constructed of 4,332 atoms interacting under a truncated Lennard-Jones potential. The film was equilibrated at temperature of \( \frac{k_B T}{\epsilon} = 1 \times 10^{-12} \text{K} \) where \( k_B \) is Boltzmann's constant and \( \epsilon \) is the well depth in the potential. Two projectiles composed of 271 and 542 particles were also equilibrated using the same potential at the same temperature. The length of the two projectiles were such that the aspect ratios were 1 to 1 and 2 to 1 respectively. For each of the projectiles two impact velocities at normal incidence were considered. The first of these had a velocity of \( 20\sqrt{\epsilon/m} \), and the second impacted at a speed of \( 40\sqrt{\epsilon/m} \) where \( m \) is the mass of the molecule. These correspond to velocities of approximately 3 to 6 km/sec. The temperature and pressure were calculated using the expressions:

\[
T(t) = \frac{1}{3k_B N} \sum_{i=1}^{N} m v_i(t)^2 ,
\]

where \( T(t) \) is the temperature \( N \) is the number of particles, \( v_i \) is the velocity of the \( i \)th particles and

\[
P(t) = \frac{N k_B T(t)}{V} + \frac{1}{6V} \sum_{i<j} \left[ r_i(t) - r_j(t) \right] \cdot F_{ij}(t) ,
\]

where \( P(t) \) is the pressure, \( V \) is the volume \( r_i \) is the position of the \( i \)th particle and \( F_{ij} \) is the force between the \( i \)th and \( j \)th particles. In addition to the normal incidence mentioned above, oblique impacts at 45° angles have also been studied for the two different aspect ratios at an impact speed of approximately \( 28\sqrt{\epsilon/m} \) (\( \sim 4.5 \text{ km/sec} \)).

Conclusions: The time evolution of the pressure, temperature, and density as shown in Figs. 1-3 will be studied for a series of hypervelocity events including those mentioned above. The presentation will include a study of the propagation of the temperature and pressure waves in the thin film as it undergoes the impact. Additional consideration will be given to the change in velocity as seen by the projectile. From this study MD will be shown to be an effective way to increase the present understanding of hypervelocity events.

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a) Plot where the aspect ratio was 1 to 1 and the natural velocity was 20 (~3.1 km/sec).

b) Plot where the aspect ratio was 1 to 1 and the natural velocity was 40 (~6.2 km/sec).

c) Plot where the aspect ratio was 2 to 1 and the natural velocity was 20 (~3.1 km/sec).

d) Plot where the aspect ratio was 2 to 1 and the natural velocity was 40 (~6.2 km/sec).

Figure 1a-1d A two dimensional representation of the time evolution of density in a thin film as the film undergoes a hypervelocity impact with normal incidence. There were 4332 particles in the thin film interacting under a truncated Lennard-Jones potential. The projectile was composed of 271 particles for the 1 to 1 impacts, and 542 particles in the 2 to 1 impacts. Each of the frames is separated by a 25 time steps with each time step being one hundredth of a picosecond. The darker areas refer to regions of high density, while the light regions have low density.

Figure 2 Plot of the time evolution of the temperature with units kT/ε for the entire film undergoing a hypervelocity impact.

Figure 3 Plot of the time evolution of the pressure with units PV/ε for the entire film undergoing a hypervelocity impact.