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SHOCK WAVES IN CONDENSED MATTER

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Molecular Dynamics Simulation of Shock Waves in Boron Nitride Nanotubes

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Shock on boron-nitride nanotubes is molecular dynamics simulated using original interatomic potentials in comparison with shock compacting of metallic nanoparticles. Vibrations during shock are modelled by nanotubes compression. At low compressions the calculated Fourie-spectra consist of one or a few dominant optical harmonics depending on atoms positions. At high compression the acoustic vibrations generated during shock are shown to transform into amorphization and fracture of nanotubes.

NUMERICAL SIMULATION OF PLASMA JETS CONTAINING SHOCKS AND MACH DISKS

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Introduction

Knowledge of the plasma jet structure is important to several areas of applications, such as plasma spraying, detonation spray process, jet propulsion efficiency, etc. Jet flow structure is determined by nozzle exit pressure, temperature, and Much number and contains a rich combination of flow interactions and physics.

These include turbulent mixing and compressibility effects such as rarefactions and shocks. Jet exit pressure can differ from ambient pressure. This pressure difference between the plasma jet and the ambient gas is resolved locally by Mach disks inside the jet. Mach disk formation can occur in both overexpanded and underexpanded jets. The main purpose of this contribution is to present a method for plasma flow prediction using high-resolution shock-capturing Total Variation Diminishing (TVD) schemes. Although the jet flow may contain a variety of complex flow physics features, the TVD method simply requires that the initial and boundary conditions to be specified for the problem. Detailed plasma flow physics developments in the jet are predicted reasonably by the TVD method. The validity of this approach is demonstrated by the high quality jet flow solutions.

Model and Numerical Method

The motion of the plasma jet is governed by the conservation laws of mass, momentum, and energy and is described by Eulerian approach. The mathematical model developed is based on the following assumptions: 1) the plasma jet is time-dependent; 2) the gas in the plasma jet is compressible; 3) the flow is laminar; 4) the plasma is continuous and in the state of local thermodynamic equilibrium; 5) the plasma jet has azimuthal symmetry and the governing equations are two-dimensional in the axisymmetric coordinate system. The governing equations are the three classic gasdynamic equations, defined as follows:

$$\begin{aligned}
&\frac{\partial\rho}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}(r\rho u)+\frac{\partial}{\partial z}(\rho v)=0\\
&\frac{\partial\rho u}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho u^2\right)+\frac{\partial p}{\partial r}+\frac{\partial}{\partial z}(\rho u v)=0\\
&\frac{\partial\rho v}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}(r\rho u v)+\frac{\partial}{\partial z}\left(\rho v^2+p\right)=0\\
&\frac{\partial E}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}(r u(p+E))+\frac{\partial}{\partial z}(v(p+E))=0
\end{aligned}\qquad(1)$$

where ρ is the density, u and v are the radial and axial velocities, $E=\rho I+\frac{1}{2}\rho(u^2+v^2)$ is the total energy per unit volume, p is the pressure, I is the specific internal energy. In our model, the equations of state are precalculated for a density-temperature grid and table interpolation is used in the hydrodynamics code. For calculation of the characteristics of plasma ions and atoms the Hartree-Fock-Slater system of quantum mechanical equations is solved. Calculation of ionization balance and charge states is performed within the collisional radiative model. Calculated values are used to determine the equations of state. The plasma pressure is expressed as $p=k(T_i\sum_k n_k+T_e n_e)-P_c$, where n_k is the number density of k-ions, n_e is the number density of free electrons, P_c is the Coulomb correction to the plasma pressure at high density and low temperature, k is the Boltzmann constant. The summation is performed over all the types of ions existing in the plasma. The plasma specific internal energy is expressed as

$$I = \frac{3k}{2\rho}\left(T_i \sum_k n_k + T_e n_e\right) + \frac{1}{\rho}\sum_k n_k (Q_k + \varepsilon_k) - E_c, \qquad (2)$$

where E_c is the Coulomb correction to the plasma internal energy at high density and low temperature, ε_k is the mean excitation energy of k-th ion, Q_k is the sum of ionization potentials from neutral atom to $k-1$-th ion.

It is known that numerical results could be strongly affected by the features of the numerical schemes employed in simulation of the convective fluxes. The governing Eqs. (1) are solved using the high-resolution TVD scheme [1]. It utilizes a Roe-type linear Riemann solver [2] by making a decomposition in the characteristic wave fields. The gasdynamic Eqs. (1) are discretised in space by an explicit second-order-accurate TVD scheme and in time by a two-stage predictor-corrector scheme which is second-order accurate in time. The TVD scheme ensures that the numerical total variation of the discretised conservative variables does not increase with time, thus no spurious numerical oscillations are generated. This TVD property is achieved by applying the slope limiters on the jumps allowed in each of the characteristic wave fields. The more diffusive minmod limiter [3] is used as it is more robust and maintains positivity of pressure and density better than the sharper limiters. It allows to achieve the TVD property close to discontinuities and sharp gradients.

Results of the Numerical Simulation

It is assumed that the argon transonic jet exits the nozzle with diameter of 8 mm into a cold atmosphere at normal conditions. A rectangular mesh was used, subdivided in a uniform 160x120 grid. The length of the calculation domain was 80 mm and its radius 30 mm. At the nozzle exit, the following profiles were used for the temperature and the axial component of the velocity [4]

$$T = T_a + (T_m - T_a)\left(1-\left(\frac{r}{R}\right)^{4.5}\right) \text{ and } v = v_m\left(1-\left(\frac{r}{R}\right)^{2}\right), \qquad (3)$$

where T_m and v_m are the velocity and temperature on the jet centerline at the nozzle exit, T_a is the temperature of the anode wall, set to 700 K, R is the nozzle radius. In accordance with measurements [5] the T_m and v_m values were taken as 13000 K and 1800 m/s, respectively. At the inlet the profiles (3) are used for the temperature and the axial component of the velocity. The initial pressure at the inlet is set equal to 8 atm. At the nozzle exit the conditions of the continuity of density and axial and radial velocities are applied. The remaining part of the nozzle exit plane as well as the substrate is considered as a wall. The other boundaries are assumed free.

As the high velocity plasma jet exits the nozzle into a stagnant atmosphere its internal energy is transformed into the kinetic energy of the entrained air. Part of

the initial kinetic energy of the jet is also transferred to the surrounding medium. It leads to the development of highly complex flow in ambient air. Fig. 1 shows the counters of temperature, pressure, density and two-dimensional velocity distribution at 250.01 μs. It is seen that the plasma flow develops a shear layer at the outer edge of the jet. This shear layer is rolling up into a ring vortex which is pulled downstream by the plasma flow. During the roll-up process, the entrainment of the surrounding air into the potential core of the jet takes place. This effect will be more pronounced with account of the turbulence in our model.

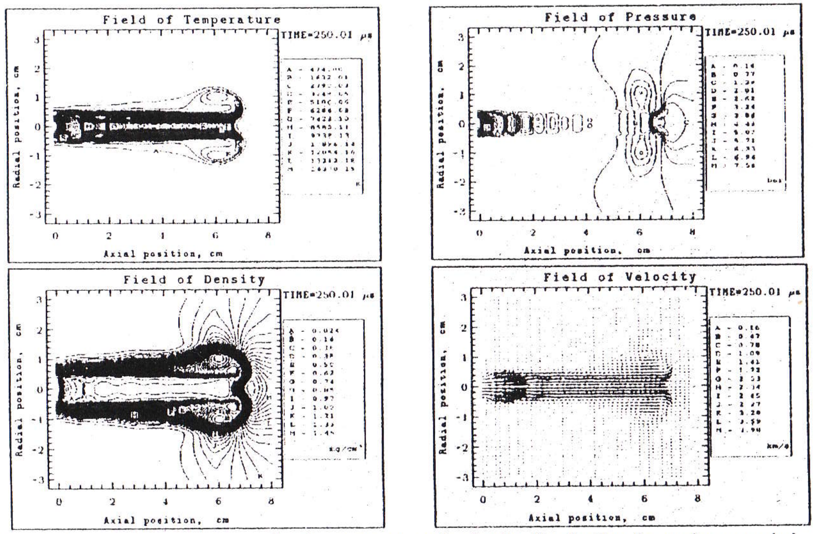

Fig. 1. Temperature, pressure, density contours and velocity distribution for underexpanded plasma jet containing multiple Mach disks at time 250.01 μs.

The flow at the inlet is high subsonic with exit Mach number 0.92. Due to transformation of the internal jet energy into the kinetic one, the velocity rapidly increases from the nominal velocity at the inlet to a peak value near the nozzle exit. The shock fronts are clearly defined in Fig. 1 by the pressure contours. At the jet exit a curved shock is formed to resolve the pressure difference between the flow inside the jet and the ambient gas. The pressure distribution of the underexpanded jet is characterized by a sharp shock front and pressure peak close to the jet exit. A well-formed Mach disk is located close to the nozzle exit. The radius of the Mach disk is approximately 0.9 cm. The Mach number downstream of the first Mach disk has accelerated to value greater than 3.5. The flow after the first Mach disk becomes subsonic. The Mach number is reduced to values below 0.6. High static pressure after the first Mach disk immediately leads to rapid acceleration and expansion of the subsonic flow. A second Mach disk is subsequently formed at 1.8

cm. Downstream of the second Mach disk, the flow accelerates to supersonic speeds with Mach number near 1.3. The consequence of Mach disks which are much weaker is further generated along the jet centerline.

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FORMATION OF DUST CLOUD AND BLAST WAVE EFFECTS AT HIGH-YIELD VOLCANIC ERUPTIONS

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Model of Volcanic Explosion

The physics model is based on separate description of the processes of dust transportation and dynamics of perturbed area. Characteristics of cold atmosphere (density and pressure as a function of atmosphere height) are determined using the CIRA-86 model [1]. The model of dust cloud formation and transportation is based on three basic assumptions. First, it is supposed that dust particles are moved with a velocity equal to local airflow one. Second, the reliable evaluations of state of dust environment can be made in the assumption that gasdynamic fields are the same as in the absence of dust. And finally, the motion of any dust particle or particle group does not depend on the presence either motion of any other particle or particle group.

For difference approximation of gasdynamic equations in space the explicit second order accuracy TVD-scheme [2] is used. For transition from n-th time step to n+1-th the two-stage second order in time Runge-Kutta TVD-scheme [3] is applied. The merit of the TVD-schemes is that they allow with a good accuracy to investigate gasdynamic flows the velocity of which is less the characteristic sound velocity. The problem is considered in a three-dimensional Cartesian coordinate system. It is supposed that the axes X1 is directed upwards, the axes X2 - to the right, and the axes X3 is perpendicular to the plane (X1,X2). The plane (X2,X3) corresponds to the ground surface. The half-space X1>0 is occupied by the atmosphere. The source of energy liberation is placed on the plane (X2,X3). The calculation of gasdynamic characteristics is performed on an irregular grid the size of which is determined by the area of air perturbed by motion. At reaching by the airflow of one of the grid boundaries the increase of cell sizes using the law of geometrical progression with a specific factor is performed.

Model of Particles-Representatives

Volcanic ashes are considered as a polydispersible particle system of specific mass. The set of dust particles localized in some area and close in characteristics is represented as one particle-representative [4]. The mass of representative is determined to equal the total mass of the whole set of the same type dust particles. The state of each representative is defined using the specification of three spatial coordinates, three velocity components and mass. The transportation of representatives is simulated on the basis of the Monte-Carlo method. For this purpose the displacement in space during a small time interval is determined as a random function of local gasdynamic velocity and velocity which the representative gains due to gravity. Action on the dust particles of air turbulence is also taken into account using the semiempirical diffusivity. The mass distribution of representatives on sizes is determined using the lognormal law with constant dispersion and median.

Results of Numerical Simulation

Initially, it is supposed that the liberated energy is contained in the thermal energy of gas with the temperature about 1700 K, density $1{,}29\cdot10^{-3}$ g/cm^3. This gas occupies the hemispherical volume with a specified radius. In consequent times the expansion of hot area into the inhomogeneous atmosphere is considered. To describe the dust particles in the range of diameters from 0,2 microns up to 2 mm, 20 discrete sizes of particles (groups) are used. The number of particles-representatives in each of the groups is taken to equal 4000. The area of space contained in one quadrant is only considered as the problem is symmetrical with respect to the vertical axes X1. The gasdynamic equations are approximated in the computational domain with a grid having 80x80x80 cells.