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Modeling of carbon laser produced plasma expansion in nitrogen environment

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Abstract

We are interested by the study of the hydrodynamic expansion of a plasma in vacuum or gas ambiance. We propose a method to deal with the compressible vapour expansion of the plasma by numerically solving the Navier-Stokes equations. A radiation term du to the plasma emission is taken into account in the energy equation, by introducing a radiation transfer equation (RTE). The finite volume method is used to discretize the Navier-Stokes equations.

1. Introduction

During the interaction of a pulsed laser beam (excimer laser) with a carbon target surface, a vapour or plasma composed of electrons, carbon ion species and neutrals undergoes an expansion into a target chamber, as shown on figure (1). The chamber could be put in vacuum conditions or filled by a given gas. In the case of the nitrogen gas, the aim is to obtain thin films of CN material that could be deposited on substrates, and the process is called pulsed laser deposition (PLD).

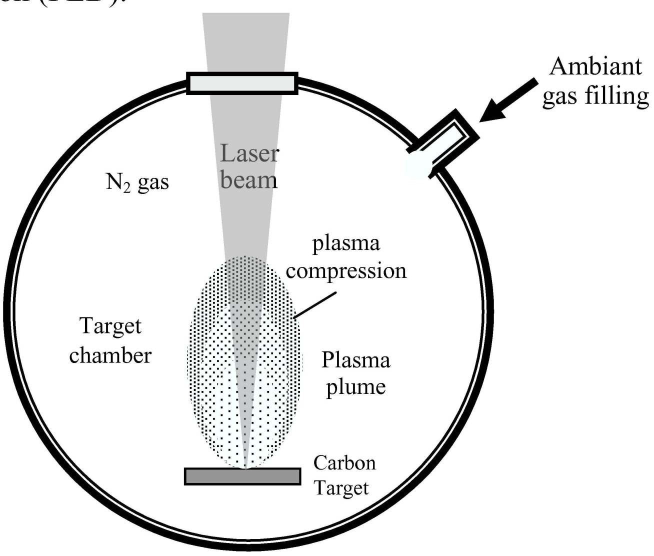

Fig. (1)

Beyond the discontinuity [1] separating the vapour phase from the fused material region, the plasma can be considered as an ideal gas.

In their paper, Ho *et al.* [2], have studied by numerical simulation, the interaction of pulsed laser irradiation of nanosecond duration with a metal surface. The compressible gas dynamics is computed by solving a system of Euler equations. In our contribution, we consider a dissipative term due to the plasma viscosity and then the dynamic of the compressible vapour (plasma) is treated by solving a Navier-Stokes equations system composed of the mass, the momentum, and the energy conservation equations.

2. The Hydrodynamic Equations

The equations describing the plasma expansion is given in the set (1-3), which is supplied by an equation of state (4) in the isentropic case.

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}(\rho v_i)=S_m \tag{1}$$

$$\frac{\partial}{\partial t}(\rho v_i)+\frac{\partial}{\partial x_j}(\rho v_i v_j)=-\frac{\partial p}{\partial x_i}+\rho g_i+\frac{\partial \tau_{ij}}{\partial x_j}+F_i \tag{2}$$

$$\frac{\partial}{\partial t}(\rho E)+\frac{\partial}{\partial x_i}(v_i(\rho E+p))=\frac{\partial}{\partial x_i}(-q+v_j\tau_{ij})+S_h \tag{3}$$

$$p=(\gamma-1)\rho E \tag{4}$$

ρ is the density, v_i the velocity component, p the pressure, ρg_i and F_i are the gravitational body force and external body forces. S_m and S_h are source terms, q the heat quantity, τ_{ij} the stress tensor describing the dissipation of energy due to the plasma viscosity.

3. Laser-plasma coupling

When an intense laser pulse interacts with metal vapor, an amount of laser energy is absorbed by the ionized particles. Whereas an emission of radiation by the plasma may couple strongly with the plume hydrodynamics. The laser-plasma coupling is represented in the equations by the S_h laser energy absorption term and the cooling term given by $\frac{\partial}{\partial x_i}(-q)$.

3.1. Plasma emission of radiation

The cooling term can be expressed as a function of the Planck mean absorption coefficient k_{pl}, the black body intensity I_b, and the solid angle, such as:

$$\frac{\partial}{\partial x_i}(-q)=-\,k_{pl}\,(4\pi\ _b-\int_{4\pi} I\,d\Omega) \tag{5}$$

Where I is the radiative intensity, which is calculated by introducing the radiative transfer equation (RTE). The RTE for an absorbing, emitting, and scattering medium at position $\vec{r}$ in the direction $\vec{s}$ is :

$$\frac{dI(\vec{r},\vec{s})}{ds} + (a+\sigma_s)\, I(\vec{r},\vec{s}) = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi}\int_0^{4\pi} I(\vec{r},\vec{s}')\, \Phi\,(\vec{s}.\vec{s}')\, d\Omega' \quad (6)$$

where $\vec{r}$ is the position vector, $\vec{s}$ the direction vector, $\vec{s}'$ the scattering direction vector, s the path length, a the absorption coefficient, n the refractive index, σ_S the scattering coefficient, the Stefan-Boltzmann constant, I the radiation intensity, which depends on position ($\vec{r}$) and direction ($\vec{s}$), T the local temperature, Φ a phase function, and Ω' the solid angle. $(a+\sigma_S)s$ represents the optical thickness or opacity of the medium. The refractive index n is important when considering radiation in semi-transparent media.

3.2. The laser energy absorption

The inverse bremsstrahlung is supposed to be the main absorption mechanism of laser radiation by the plasma. Then S_h is taken as:

$$S_h = k_p\, I_{inc} \exp\left(-k_p\, |z|\right) \quad (7)$$

Where k_p is the laser energy absorption coefficient by the plasma, and I_{inc} the incident laser intensity.

3.3. The ionization states

The ionization rates are calculed by the mean of Saha-Eggert equation [eq.(8)] that gives the density of ions species as a function of the temperature. In our case we suppose a local thermodynamic equilibrium (LTE) condition.

$$\frac{n_e\, n_i}{n_n} = \frac{2(g_o)_i}{(g_o)_n} \frac{(2\pi\, m_e\, kT)^{3/2}}{\hbar^3} \exp\left(\frac{-W_i}{k_B T}\right) \quad (8)$$

n_e, n_i et n_n are the electron, ion, and neutral densities, g_o is the state statistic weight, m_e the electron mass, k_B the Boltzmann constant, and W_i the ionization energy. The densities are given in (particule/cm^3), and they are related by the relation:

$$n_e = \sum_i Z_i n_i \tag{9}$$

The density of the vapour given in (g/cm^3) is related to n_n and n_i by:

$$\rho = \frac{M}{N_a}\left(\sum_i n_i + n_n\right) \tag{10}$$

where M is the atomic mass of the target material, and N_a the Avogadro number.

4. The numerical solution

The treatment of the Navier-Stokes equation is performed numerically after transforming the PDE equation system (1-4) to a form that allow a discretization by finite volume method. A set of algebraic equations is thus obtained and solved by the known numerical methods. Discretization of the governing equations can be illustrated most easily by considering the steady-state conservation equation for transport of a scalar quantity Φ. This is demonstrated by the following equation written in integral form for an arbitrary control volume V as follows:

$$\oint \rho\phi\vec{v}.d\vec{A} = \oint \Gamma_\phi \nabla\phi.d\vec{A} + \int_V S_\phi\, dV \tag{11}$$

Equation (10) is applied to each control volume, or cell, in the computational domain. Discretization of Equation (10) on a given cell yields

$$\sum_f^{N_{faces}} \rho_f \vec{v}_f \phi_f . \vec{A}_f = \sum_f^{N_{faces}} \Gamma_\phi (\nabla\phi)_n . \vec{A}_f + S_\phi V \tag{12}$$

where N_{faces} is the number of faces enclosing cell, ϕ_f the value of Φ convected through face f, $\rho_f \vec{v}_f . \vec{A}_f$ the mass flux through the face, $\vec{A}_f$ area of face f, ($|\vec{A}| = |A_x\vec{i} + A_y\vec{j}|$ in 2D), $(\nabla\phi)_n$ the magnitude of $\nabla\phi$ normal to face f, V the cell volume.

References

[1] C.J. Knight , AIAA Journal, 17 (5), 519, 1979.

[2] J.R.Ho, C.P.Grigoropoulos, and J.A.C.Humphrey, J. Appl. Phys. 79 (9)1996.