Influence of the nonequilibrium distribution function on dynamics of gas-surface scattering

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Abstract

We considered different aspects of interaction gas with aluminum plate. Computer simulation by dynamic methods of nonequilibrium gas and surface molecules interact in little district (2.5 of the lattice constant of the crystal structure) near surface. The distribution function is reconstructed. We investigate the long tail of destruction function on process of taking out molecules from surface.

Keywords: Boltzmann equations, Chapman-Enskog method, conjugate problem the Navie-Stokes, the molecular dynamics method.

1 Introduction

The important question for the problem of layer near a moving spacecraft is boundary conditions. It is necessary to know aerodynamic characteristics. These conditions are known badly for rarefied gas and for turbulence streams. To solute the Boltzmann equation is more difficult than Navier-Stokes equations. So better to solute Navier-Stokes equations. Usually for the classical case near the surface the Knudsen layer is considered. This layer has the length of order free path. M. Lunc, J. Luboncki, V.C.Liu , R.G. Patterson, W. Bule, F.O.Goodman, H.Y.Wachman, R G. Barantsev, Yu. A.Ryzhev, G.V. Dubrovskii and the others investigated the interaction molecules with surface near freely-molecular simulations. At present majority experimental and theoretical results were received for dispersion of monovelocity beam of atoms. Conjugated conditions at surface without the Knudsen layer are written to count friction and heat flow to the surface by solution the Boltzmann equation without collision integral in thin layer and by solution the Navie-Stokes equations with addition new terms with influence of an angular momentum variation in an elementary volume. The boundary conditions are made more accurate for rarefied gas and for transition flow regime. The molecular dynamics method is used to investigate the influence of the profile of the equilibrium distribution function on the exfoliation of the surface layer of aluminum for moving surface. This is the first step.

2 Influence of the dispersion near the surface

The problem for moving gas near the surface has some singularities. The modified Boltmann and Navier-Stokes equations are needed boundary conditions. To solute the Boltzmann equation is more difficult than Navier-Stokes equations. So better to solute Navier-Stokes equations [1-9]. In our case the equation for two-part distribution function near the

surface is

$$\frac{\partial f_2}{\partial t}+\sum_{i=1}^{2}\left\{\xi_i\cdot\left[\frac{\partial f_2}{\partial x_i}\right]+\xi_i\cdot\frac{\partial}{\partial x_i}\left[x_j\frac{\partial f_2}{\partial x_j}\right]-\frac{X_i}{m}\frac{\partial f_2}{\partial \xi_i}\right\}+X_{12}\cdot\frac{\partial f_2}{\partial \xi_1}+X_{21}\cdot\frac{\partial f_2}{\partial \xi_2}+X_{22}\frac{\partial f_2}{\partial \xi_2}=0.$$

Integrating in ξ we obtain the equation for one-particle distribution function with interaction force gas molecule with surface molecules. Suggested algorithm is easily than classical. For ξ_2= 0 in solid body (without movement of the surface molecules) we have trajectory problem i.e. the usual of DSMC code**.**

3 The method of investigation

To simulate the interaction of gas with the crystal surface method has been applied molecular dynamics (MD), based on the solution of the equations of Newton [10]. In the first stage of modeling is the initial distribution of particles in space (spatial configuration of the crystal structure and the gas phase) and initial distribution of particle velocities corresponding to the mechanical and thermal motion of the system in the initial state. The generation of initial conditions occurs at the macro and micro levels. At the macroscopic level, wondered the geometric dimensions of the area in which calculations were carried out (L_x, L_y, L_z) and the macroscopic velocity. Under the macroscopic velocity of the bombarding mean directional velocity of the gas stream. At the microscopic given level of packing particle structure (fcc lattice of the crystal surface) and the velocity distribution of the thermal motion of gas particles and the crystal structure. The thermal velocity distribution at the initial time is generated according to the Maxwell distribution

$$\mathrm{f}\,(\upsilon)=\frac{4}{\sqrt{\pi}}\left(\frac{m}{2kT}\right)^{3/2}\upsilon^2 e^{-\frac{m\upsilon^2}{2kT}}$$

where m is mass of atom, k is Boltzmann constant and T gas temperature.

The rate of gas particles at the initial moment of time is made up of directed macroscopic velocity and thermal velocity. The second stage computes the values of the coordinates and velocities of particles (describing the evolution of the system over time), which were carried out using the MD equations of motion integration algorithms with predetermined conditions based on the scheme Varlet [10]. The time step was chosen to be 5 fs, which is comparable with the period of molecular vibrations of the lattice.

The trajectories of the particles were calculated in a macroscopic ensemble under the thermodynamic conditions: constant number of particles, constant volume and constant temperature. The constancy of temperature in the system provides an introduction Noze-Hoover thermostat [12]. The number of gas particles was chosen to be 25, which corresponds to the pressure 1 atm in the computational volume 10^6 ang. at 290 K. The number of particles in the structure of the computational domain is chosen equal to 10000. In this paper, the interaction between particles of type structure-structure described by a Morse potential [11]

$$U\left(r_{ij}\right)=D_0\left[e^{-2\alpha(r-r_0)}-2e^{-2\alpha(r-r_0)}\right],$$

where r_0 is the equilibrium internuclear separation and D_0, The well depth, is the dissociation energy of the molecule, α is an adjustable shape parameter.

For particles such as gas-gas and gas-structure described by Lennard-Johnes potential

$$U\left(r_{ij}\right) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right],$$

where ε is well depth σ is affective atom diametr.

The potential parameters for the structure of the gas-particles were calculated using the formula [10]

$$\sigma_{gs} = \frac{\sigma_g + \sigma_s}{2}$$

and

$$\varepsilon_{gs} = \sqrt{\varepsilon_g + \varepsilon_s}$$

Theqradius of the particle interaction is chosen to be 2.5 of the lattice constant of the crystal structure.

Due to the limited computing resources the distribution function of gas particles is divided into a region of the velocities. For each region MD calculation was processed and distribution function was reconstructed (Fig. 1). Some particles due to the directional velocity received energy that enough to penetrate into the crystal structure (Fig. 2).

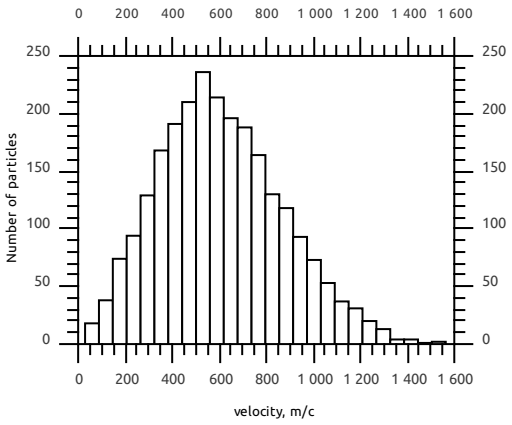

Figure 1: Gas distribution function

Conclusion

Verified the absence of collisions between a gas in a narrow layer adjacent to the surface even for the normal pressure. Displaying the introduction of the gas molecules and the presence of fatigue effects in the case of directional velocity at the outer boundary. Proved the possibility of rejection of the Knudsen layer.

References

[1] S. V. Vallander. The equations for movement viscosity gas. DAN SSSR .1951. V. LXX šššš, N 1

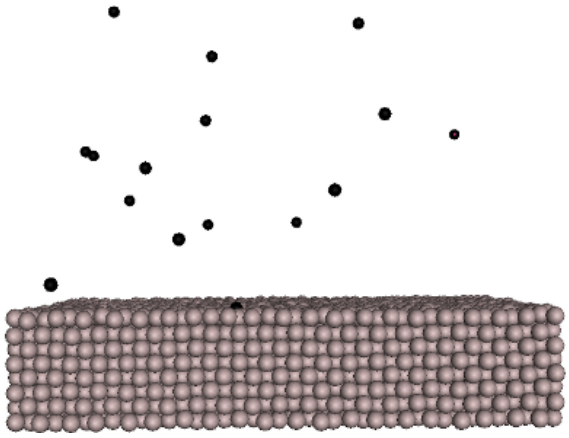

Figure 2: Penetration atom into crystal structure

[2] Alexeev. Generalized Boltzmann Physical Kinetics. Elsevier, Amsterdam, 2004

[3] C. Cercignani, Mathematical methods in kinetic theory Macmillan. 1969

[4] J.H. Ferziger, H.G. Kaper, Mathematical theory of transport processes in gases./ Amsterdam-London.1972.

[5] J.O. Hirschfelder, C.F. Curtiss, R.B. Bird, The molecular theory of gases and liquids. New-York, 1954.

[6] M.N. Kogan, The dynamics of the rarefied gases. M.: Nauka, 1967.(Russian)

[7] E.V. Prozorova, *Influence of dispersion in mechanics*. Seventh International Workshop on Nondestructive testing and Computer Simulations in Science and Engineering, edited by Akexander I. Melker, Proceedings of SPIE Vol.5400 (SPIE, Bellingham, WA, 2004) pp.212-219.

[8] E.V.Prozorova. Influence of the dispersion in nonequilibrium models for continuous mechanics. Proceedings of XXXVIII Summer School "Advanced Problems in Mechanics", pp. 568-574, Spb. 2010

[9] E.V. Prozorova. Influence dispersion and cross flux in continuous mechanics. THE EUROPEAN conference for aerospace scinces. (Russia, Saint Petersburg, 2011), id365 www.eucass.ru/cs/upload/gF76bMq/papers.zip

[10] M. P. Allen and A. K. Tildesley Computer Simulation of Liquids. – Oxford: Clarendon Press. 1987

[11] L. A. Girifalco, G. V. Weizer Application of the morse potential function to cubic metals // Phys. Rev. 114(3): p. 687 1959

[12] W. G. Hoover Cononical dynamics: Equilibrium phase-space distribution // Phys. Rev. A. 1992 V. 31. P. 1695-1697