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The accommodation coefficients, which characterize energy and momentum transfer in the problem of the interaction of a rarefied gas with a surface, can be calculated by analytical or numerical methods in which the initial disturbances of the crystal lattice are taken into account or ignored. This necessitates replacement of the infinite three-dimensional crystal of the solid, depending on the approximate formulation of the problem, by a finite one-, two-, or three-dimensional assembly of atoms connected by particular bonds or without such bonds. The accuracy of the result when this replacement is made has to be assessed.

In [1] the zones of free movement and strong interaction in a two-dimensional model were determined, and in [2] estimates were made of the length of the chain of atoms involved in the collision act in the one-dimensional case. In this paper we investigate the effect on the accommodation coefficients of the size of the block of solid atoms which are implicated in the collision and are taken into consideration in the case of interaction of a gas atom with a surface.

In the one-dimensional problem all the atoms of the chain at the initial instant have random (in direction and magnitude) displacements from the equilibrium position and vibration velocities.

The dependence of the energy and momentum accommodation coefficients on the initial conditions and gas parameters is determined, and the number of atoms in the chain which affect the accuracy of calculation of the accommodation coefficients for a prescribed interaction energy is estimated.

In the two- and three-dimensional cases the forces of interaction of the surface atoms with the incident gas atom are estimated. With increasing distance from the target atom the forces diminish, and, hence, it makes sense to obtain information about the number of surface atoms which are directly implicated in the collision act, in addition to the target atom, and affect the value of the accommodation coefficients.

After the appropriate evaluations the solid can be regarded as a finite three-dimensional crystal. We describe the method and the scheme of calculation of the energy and momentum transfer between the rarefied gas and the solid surface.

The atoms in the lattice are connected with one another by elastic forces proportional to the displacements from the equilibrium positions. The displacements and velocities of the atoms in the crystal at the initial instant, defined as the start of interaction with the gas

atom, have random magnitude and direction. The gas atoms have a macrovelocity which corresponds to an interaction energy of ~5-10 eV, and have a Maxwellian thermal-velocity distribution. The interaction is assumed to be collective, i.e., at the individual gas atom collides with the whole block of solid atoms. The individual accommodation coefficients are calculated in relation to the initial position and velocity of the gas atom. The values are averaged over the parameters which determine the initial state of the interacting system and the corresponding averaged accommodation coefficients are calculated. The interaction between the gas and crystal atoms conforms to the Lennard-Jones law [the (6-12) potential is used in the calculations].

1. The system of equations of motion for the gas atom and the linear chain of solid atoms interacting through the potential  $\phi(x_1)$  can be written in the form (see [3, 4]):

$$\begin{aligned} \ddot{x}_0(\tau) &= \frac{1}{k\mu} \frac{d\phi(x_1)}{dx_1}, & \dot{x}_2(\tau) &= \frac{1}{k} \frac{d\phi(x_1)}{dx_1} - \frac{1}{2} x_3(\tau), \\ \dot{x}_1(\tau) &= 1/2 [x_0(\tau) - x_2(\tau)], \\ \dot{x}_n(\tau) &= 1/2 [x_{n-1}(\tau) - x_{n+1}(\tau)] \quad (n \geq 3). \end{aligned} \tag{1.1}$$

Here  $k$  is the constant of the force of interaction between the links of the chain;  $\mu$  is the ratio of the masses of the gas and chain atoms;  $\tau$  is the reduced time;  $x_{2n+1}(\tau)$  and  $x_{2n}(\tau)$  and  $x_{2n}(\tau)$  are, respectively, twice the relative displacement of the  $n$ -th and  $(n+1)$ -th atom and the velocity of the  $n$ -th atom. We assign a (6-12) Lennard-Jones potential to the interaction of the gas atom and the first atom of the chain and put  $\alpha^0 = 2\epsilon/\sigma^2k$ .

We assume that all the displacements are referred to  $a/2$ ;  $a$  is the lattice spacing;  $\epsilon$ , and  $\sigma$  are parameters of the Lennard-Jones potential. We take the positive direction along the chain axis as the direction towards the gas atom and assume that the zone of free motion is a distance of  $2a$  from the equilibrium position of the first chain atom and the maximum amplitude of the lattice point does not exceed  $a/2$ , so that the relative displacements of the points will be in the interval  $[-1, \dots, 0, \dots, +1]$ . Since the model is suitable only for small displacements, this interval in the initial conditions is reduced by an order. In relative magnitudes the range of variation of the velocities of the lattice atom velocities will be included in the same interval.

Table 1

l	$\mu$	$\alpha^0$	n = 6			n = 10		
			$\alpha_n$	$\alpha$	(1) <sup>*</sup>	$\alpha_n$	$\alpha$	(2) <sup>*</sup>
10	0.1	0.01	0.170	0.310	5	0.169	0.309	5
10	0.3	0.01	0.334	0.556	4	0.329	0.550	
10	0.5	0.01	0.608	0.846		0.677	0.887	
10	0.9	0.01	0.910	0.992	3	1.000	1.000	1
10	0.1	0.1	0.288	0.493	1	0.273	0.472	
10	0.3	0.1	0.580	0.723	2	0.591	0.832	
10	0.9	0.1	0.966	0.999		0.926	0.995	
100	0.9	0.1	0.899	0.990		0.899	0.989	
100	0.1	0.01	0.088	0.165		0.084	0.161	4
100	0.5	0.01	0.691	0.905		0.680	0.898	2
100	0.1	0.001	0.052	0.100		0.052	0.101	
100	0.3	0.001	0.240	0.422		0.246	0.431	
100	0.5	0.001	0.535	0.784		0.530	0.778	
100	0.9	0.001	0.870	0.983		0.854	0.979	
500	0.5	0.01	0.590	0.830		0.592	0.834	3
500	0.5	0.001	0.535	0.785		0.537	0.786	

\*These columns give the numbers of the curves illustrated in Figs. 1 and 2.

The energy of the incident atom is prescribed by the parameter  $l$ , which is given by the equality  $Mv_0^2/2 = \epsilon l$ .

Thus, the initial conditions for system (1.1) can be written as;

$$\begin{aligned} x_0(0) &= \sqrt{l\alpha^2/\mu}, \\ x_1(0) &= 4 - \{1\}, \\ x_{2n}(0) &= \{n-1\} \quad (n \geq 1), \\ x_{2n+1}(0) &= \{n\} - \{n+1\} \quad (n \geq 1). \end{aligned} \quad (1.2)$$

Here the collision parameters are  $l$ ,  $\mu$ , and  $\alpha$ ;  $\{n\}$  denotes the set of uniformly distributed random numbers in the interval  $[-0.1, +0.1]$ .

System (1.1) with initial conditions (1.2) was solved numerically on a computer for a fixed number  $n$ . It is known that if the vibration phase of the chain atoms is ignored the energy accommodation coefficient depends significantly only on the first five atoms [2]. Hence, in the calculations we considered 6 to 20 atoms, which correspond to an order of 14 to 42 for the system of equations. The calculations were carried out for parameters  $\mu = 0.1-0.8$ ;  $l = 10-500$ ;  $\alpha = 10^{-1}-10^{-3}$  and various sets of initial conditions.

Comparative graphs of the velocities  $x_0$  of the gas atom for two values of  $n$  (6 and 10) are given in Figs. 1 and 2, respectively. The calculations show that the chain length, beginning at the sixth to seventh atom, has very little effect on the transmitted momentum and energy. The interaction time is practically unchanged. Only the qualitative picture of the vibrations of the disturbed chain (and the gas atom along with it, if capture occurs) is different when its length is different. The distant atoms are only slightly disturbed. The accommodation coefficients  $\alpha_n$  and  $\alpha$  for the normal momentum and energy for some interaction parameters are given in Table 1.

A comparison of the obtained values of the coefficients with the available results, which were not averaged, shows that the effect of the initial disturbances is independent of the chain length, and the transfer coefficients for different initial conditions are mostly close to the mean values. The chain length affects the transfer only at low interaction energies and for the gas atom velocity range of practical interest a consideration of five to six atoms in the linear model gives a high degree of accuracy.

If the light gas particles are mostly reflected with low accommodation, then in the case of interaction of heavy atoms the coefficients  $\alpha_n$  and  $\alpha$  are close to unity and at low energies the gas atom can be captured. In the last case the gas atom can complete oscillatory movements close to the surface for a fairly long time (curve 1, Fig. 2) or be captured immediately after the first oscillation (curve 3, Fig. 1).

2. In the two- and three-dimensional models, as distinct from the one-dimensional model, the potential of a given point A close to the surface is made up of the potentials of interaction with all the surface points of the lattice, i.e.,

$$\begin{aligned} \varphi(A) &= \varphi(r_0) + \sum_{n \neq 0} \varphi(r_n), \\ \varphi(A) &= \varphi(r_0) + \sum_{n, m \neq 0} \varphi(r_{n, m}) \end{aligned}$$

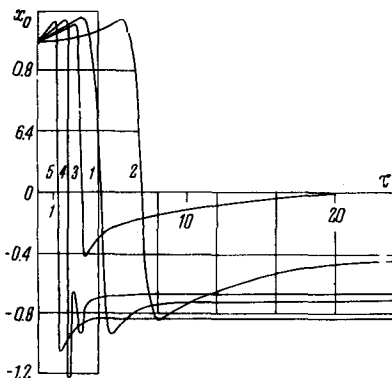


Fig. 1

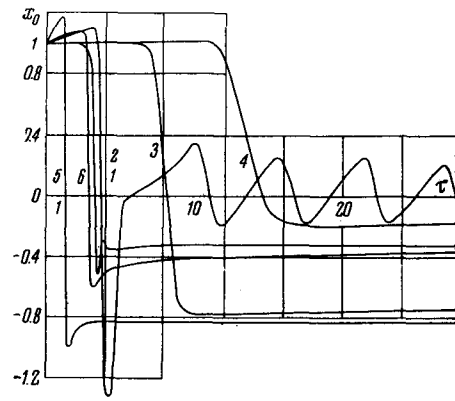


Fig. 2

in the two- and three-dimensional simple cubical model, respectively.

Here  $r_0$  is the distance to the target atom;  $n$  and  $m$  are the numbers of the neighbors. Without loss of generality, and purely for simplicity of the calculations, we will henceforth consider normal frontal collisions, and the expressions for the potential  $\varphi(A)$  will take the form

$$\begin{aligned} \varphi(A) &= \varphi(r_0) + 2 \sum_{n=1}^{\infty} \varphi(r_n), \\ \varphi(A) &= \varphi(r_0) + 4 \sum_{n=1}^{\infty} \varphi(r_n) + 4 \sum_{\substack{n>0 \\ m>0}} \varphi(r_{n, m}). \end{aligned} \quad (2.1)$$

Here  $r_n^2 = z^2 + (na)^2$ ,  $r_{n, m}^2 = z^2 + (n^2 + m^2)a^2$ , and  $z$  is normal to the surface.

It is difficult, however, to calculate analytically the sums in these expressions when  $\varphi(r)$  is replaced by a potential close to the actual one [for instance, the (6-12) Lennard-Jones potential], but this is not required, since it is sufficient to have an estimate of the interaction forces due to the distant surface atoms. Referring all the lengths to the lattice spacing  $a$  and putting the constant  $\sigma$  in the Lennard-Jones potential equal to  $a$ , the function  $\varphi(r)$  for this potential, accurate to the constant factor, will have the form

$$\begin{aligned} \varphi(r^*) &= 1/r^{*12} - 1/r^{*6}, \quad r_n^{*2} = k^2 + n^2, \\ r_{n, m}^{*2} &= k^2 + n^2 + m^2, \quad n, m = 1, 2, \dots \end{aligned}$$

Here  $k = z/a$  is the relative distance of the gas atom from the target.

Thus, for a fixed point A  $\varphi(A)$  is a function only of  $n$  in the two-dimensional case of the two variables  $n, m$  in the three-dimensional case. We investigate the first case.

We consider the partial sum  $S_n = \psi(1) + \dots + \psi(n)$  of the infinite series  $S_{\infty}$ . The residue of this series  $R_n = \psi(n+1) + \psi(n+2) + \dots$ , owing to convergence of the latter, satisfies the inequalities

$$\int_{n+1}^{\infty} f(n) dn < R_n < \int_n^{\infty} f(n) dn. \quad (2.2)$$

Here  $\varphi(r_n) \equiv \psi(n)$ , and in the improper integral  $f(n)$  will be a continuous decreasing function of  $n$ , which at  $n = 1, 2, 3 \dots$  assumes the values  $\psi(1), \psi(2), \psi(3), \dots$ .

For a specific number  $2n$  of neighbors surrounding the target atom the total potential at any fixed point close to the surface is easily calculated. The inequality (2.2) can be used to evaluate the error introduced by neglect of the effect of the more distant surface atoms. The integrals in (2.2) for the Lennard-Jones potential are calculated analytically. In what follows we need only the second one,

$$\begin{aligned} \int_n^{\infty} f(n) dn &= \left( \frac{63}{256k^{11}} - \frac{3}{8k^5} \right) \frac{\pi}{2} - \\ &= \frac{n}{10k^2(k^2 + n^2)^5} - \frac{9n}{80k^4(k^2 + n^2)^4} \end{aligned}$$

$$-\frac{63n}{490k^6(k^2+n^2)^3} - \frac{63n}{384k^8(k^2+n^2)^2} - \frac{63n}{256k^{10}(k^2+n^2)} + \frac{n}{4k^2(k^2+n^2)^2} + \frac{3n}{8k^4(k^2+n^2)} + \left(\frac{3}{8k^6} - \frac{63}{256k^{11}}\right) \arctg \frac{n}{k}. \quad (2.3)$$

In the case of interaction with a surface the evaluation of the second term in the expression for the potential function (2.1) is similar to the two-dimensional model ( $m = 0$ ), and we put the last term in the form

$$\sum_{n=1}^{\infty} \left[ \sum_{m=1}^{\infty} \Phi(r_n, m) \right] = \sum_{n=1}^{\infty} S_{nm}.$$

For this term we have the inequality

$$\int_{n+1}^{\infty} S_{nm} dn < R_n < \int_n^{\infty} S_{nm} dn$$

provided that the internal sum is calculated exactly. If we denote the residue of the internal series by  $R_m$  in an approximate calculation of the latter, then for  $R_n$  an evaluation from above in the form

$$R_n < \int_n^{\infty} \left[ \sum_{m=1}^m \Phi(r_n, m) \right] dn + \sum_n R_m \quad (2.4)$$

will be valid. If we assign  $m$  and  $n$  and fix the value of  $n$  each time we can calculate the estimates for  $R_m$ . Summing these upper limits we obtain the second term in expression (2.4). After calculation of the partial sum in  $m$  the integral in the first term is found by the usual method and summation and integration can be interchanged.

Calculations were carried out for the relative error  $\Delta R$  in the interaction potential in relation to the number of target-atom neighbors considered and are given in Table 2. The relative error in the three-dimensional model is a little higher than in the two-dimensional model, but for a small number of neighbors it is several times larger. The reduction of the error with increase in the number of neighboring atoms, however, is so rapid that for practical purposes sufficient accuracy is attained with the same number of considered neighbors in the two- and three-dimensional cases.

Comparing the calculated values of the accommodation coefficients by using the approximate cutoff potential with and without correction we note a qualitative agreement of the results, i.e., the collision of the gas atom with the wall is affected mainly by the neighbors on the surface closest to the target atom, the number of which depends mainly on the parameters of the potential and for the known potentials (including the Lennard-Jones functions) and allowance for the approximate values of the parameters themselves does not exceed two or three. The zone of free motion, however, depends mainly on the velocity of the incident gas [1].

Thus, neighboring atoms on a solid surface have less effect on energy and momentum transfer than atoms of the second and deeper layers, and the conducted calculations allow a quantitative assessment of this effect. We note that the scheme of paired interaction [1], based on distinction of a zone of strong interaction, is still valid and a consideration of the nearest neighbors at moderate velocities will give only a small correction factor to the accommodation coefficients

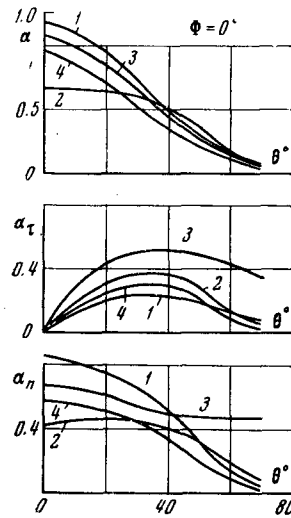


Fig. 3

calculated in [1].

3. We regard the finite block of solid atoms as a regular cubic lattice. We select one atom on the surface face and take its equilibrium position as the origin of coordinates  $(x_1, x_2, x_3)$ , where the  $x_3$ -axis is normal to this face. The lattice is struck by a flux of gas atoms with a Maxwellian distribution of velocities  $u$  and we assign to the macrovelocity a magnitude  $v$  and two angles  $\theta$  and  $\Phi$ , the first of which is measured from the normal to the surface.

Here  $\sigma$  is used as a linear scale. The initial displacements of the lattice atoms are random, distributed in relative units on the segment  $(-0.1, +0.1)$  and the maximum value of the initial velocity is determined by the binding energy of the atoms in the lattice. The position of the gas atom  $(r, \theta, \Phi)$  at the initial instant is assumed to be on a control surface separated from the plane  $x_3 = 0$  by a relative distance  $d$ , which is determined by an evaluation of the force field above the surface. In the calculations  $d$  is taken as 2, and the relative lattice spacing as  $a = 1$ . The block of atoms implicated in the collision act consists of 36 atoms. Depending on the interaction forces the control surface is divided into cells, within which the initial points are distributed uniformly.

The equations of motion for the interacting system are solved on a computer by the Adams method with a variable step.

The accommodation coefficients for the trajectory in the case of a fixed initial position of the gas atom are obtained by averaging over the velocities of this atom, which have a distribution in the form of a Maxwellian function

$$f = \left(\frac{M}{2\pi kT}\right)^{3/2} \exp \left[ -\frac{M(v-u)^2}{2kT} \right]. \quad (3.1)$$

Here  $T$  is the temperature,  $k$  is the Boltzmann constant, and the coefficients  $\alpha$ ,  $\alpha_n$ ,  $\alpha_\tau$ , which characterize the transfer of energy and momentum (normal and tangential components, respectively) between the beam of gas atoms with a prescribed macroscopic velocity and the solid, are calculated after averaging over all possible trajectories.

Table 2

$k$ $n = m$	0.5		1.0		2.0	
	$\Delta R_n$	$\Delta R_{nm}$	$\Delta R_n$	$\Delta R_{nm}$	$\Delta R_n$	$\Delta R_{nm}$
1	$0.469 \cdot 10^{-4}$	$0.937 \cdot 10^{-4}$	0.277	0.434	0.289	0.423
2	$0.271 \cdot 10^{-3}$	$0.405 \cdot 10^{-5}$	$0.318 \cdot 10^{-1}$	$0.470 \cdot 10^{-1}$	$0.733 \cdot 10^{-1}$	0.106
3	$0.385 \cdot 10^{-6}$	$0.512 \cdot 10^{-6}$	$0.522 \cdot 10^{-2}$	$0.731 \cdot 10^{-2}$	$0.202 \cdot 10^{-1}$	$0.268 \cdot 10^{-1}$
5	$0.311 \cdot 10^{-7}$	$0.372 \cdot 10^{-7}$	$0.496 \cdot 10^{-3}$	$0.595 \cdot 10^{-3}$	$0.255 \cdot 10^{-2}$	$0.306 \cdot 10^{-2}$
10	$0.102 \cdot 10^{-8}$	$0.112 \cdot 10^{-8}$	$0.165 \cdot 10^{-4}$	$0.182 \cdot 10^{-4}$	$0.101 \cdot 10^{-3}$	$0.111 \cdot 10^{-3}$
20	$0.444 \cdot 10^{-10}$	$0.466 \cdot 10^{-10}$	$0.524 \cdot 10^{-6}$	$0.548 \cdot 10^{-6}$	$0.336 \cdot 10^{-5}$	$0.351 \cdot 10^{-5}$

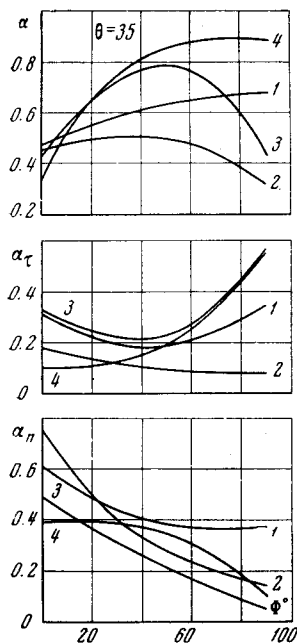


Fig. 4

All the premises and evaluations in the formulation of the problem are made on the basis of [1] and sections 1 and 2 of this paper.

The following values of parameters are used in the calculations:

$$\mu = 0.1 - 0.5, \quad \theta = 0 - 70^\circ, \quad \frac{v}{\sqrt{2kT/M}} = 8, \quad \alpha^\circ = 0.01, \\ l = 10 - 500, \quad \Phi = 0 - 360^\circ,$$

We found that at values of  $\theta > 35^\circ$  the accommodation coefficients depend strongly on the azimuthal angle  $\Phi$ . Figure 3 shows the dependences of  $\alpha$ ,  $\alpha_\tau$ , and  $\alpha_n$ , respectively, on  $\Phi$  in the range from 0 to  $90^\circ$  in the case of a fixed value of  $\theta$  ( $35^\circ$ ). We note that the dependence of the accommodation coefficients on the initial energy is different for different values of the mass ratio  $\mu$ . For instance, for  $\mu = 0.1$  the energy accommodation coefficient decreases with increase in initial energy, whereas for  $\mu = 0.3$ ,  $\alpha$  begins to depend on the orientation of the initial vector  $v$  and usually increases with increase in the parameter  $l$  for almost all  $\Phi$  and  $\theta$ . The relationship is similar for  $\mu = 0.5$ .

The coefficients  $\alpha_\tau$  and  $\alpha_n$  depend in a more complex manner on  $l$  and  $\mu$ , as can be seen in the special case and in Fig. 3. The variation of  $\alpha$  and  $\alpha_n$  with the angle  $\theta$  is shown in Fig. 4. The numerical values of  $\alpha$ ,  $\alpha_\tau$ , and  $\alpha_n$  at large  $\theta$  must be treated with caution, however, since the errors in the calculations increase with increase in  $\theta$ .

In Figs. 3 and 4 the curves are plotted for the following values of parameters  $\mu$  and  $l$ :

$$1 - \mu = 0.1, \quad l = 10; \quad 2 - \mu = 0.1, \quad l = 100; \\ 3 - \mu = 0.3, \quad l = 10; \quad 4 - \mu = 0.3, \quad l = 100.$$

The over-all qualitative picture of variation of the accommodation coefficients for the energy and tangential and normal momenta, calculated with due regard to the collectivity of interaction and averaging over the trajectories, differs a little from the picture for collective interaction without averaging [5]. For small  $\theta$  the averaged values of the accommodation coefficients are even quantitatively closer to the corresponding values for paired interaction and the same potential than the coefficients calculated in [5]. With the indicated parameters the averaged interaction time is practically independent of the selected set of parameters. In addition, the accommodation coefficients calculated for individual trajectories do not have a great spread due to the Maxwellian velocity distribution of the incident molecules (the maximum deviation from the mean value for  $\alpha$  is about 8%). This is obviously valid only for the selected range of velocities. It should be noted, however, that with increase in the angle  $\theta$  this relationship appears at velocities of the order of the first cosmic velocity and for sufficiently large angles of inclination of the incident flux to the solid surface ( $\theta \geq 70^\circ$ ) the correction to the accommodation coefficients will probably be comparable with the value of these coefficients. The calculation procedure for such angles differs from that given in this paper.

It should be noted in conclusion that a similar calculation of the averaged accommodation coefficients was carried out in [6] and agrees qualitatively with our results. In this paper, however, the formulation of the problem, the assignment of the initial conditions, and the calculation procedure differ from those in [6], mainly in the fact that practically any distribution of incident particles and fairly large angles of incidence  $\theta$  can be taken into account. In addition, superfluous information can be eliminated.

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