ENERGY EXCHANGE IN THE INTERACTION OF ATOMS WITH THE SURFACE OF AN IDEAL CRYSTAL

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Figure 1

Figure 1: Figure 1

Abstract

Full Text

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PHYSICS

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ENERGY EXCHANGE IN THE INTERACTION OF ATOMS WITH THE SURFACE OF AN IDEAL CRYSTAL

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1. At incident-atom energies of 1-20 eV, the process of its interaction with the crystal lattice of a solid may be considered within the framework of classical mechanics; moreover, at moderate temperatures the energy of thermal motion of the atom itself and of the atoms of the crystal may be neglected, while processes of sputtering of the crystal or ionization at such energies are unlikely. Below, a mathematical model of such an interaction is constructed and some numerical results are given, obtained under the following assumptions:
1) the crystal lattices (simple cubic, body-centered cubic, and face-centered cubic are considered) are Einstein lattices, i.e., they represent an ordered set of mutually uncoupled harmonic oscillators;
2) the interaction of each lattice atom with the incident atom is described by the 6-12 Lennard-Jones potential.

2. The system of equations of motion of the incident particle and of the lattice atoms and the initial conditions will include three groups of dimensionless parameters:

1) Parameters determining the properties of the particle and the initial conditions of its motion: $\bar{m} = m_1/m_2$ –relative mass; $\bar{w} = \sqrt{2E_0/\bar{m}\sigma^2\varkappa}$ –dimensionless initial velocity; φ, ψ –angles determining the direction of the initial velocity of the particle: respectively, the angle with the normal to the surface and the azimuthal angle; $\bar{x}_c = x_c/\sigma$, $\bar{y}_c = y_c/\sigma$ –coordinates of the target point on the crystal surface.

Fig. 1. Variation of the accommodation coefficient along the diagonal of the surface face of a simple cubic lattice (the x and y axes are directed along the cube edges)

2) Parameter of the interaction potential: $\bar{\varepsilon} = 24\varepsilon/\varkappa\sigma^2$ –dimensionless depth of the potential well.

3) Parameters characterizing the type of lattice: $\bar{d} = d/\sigma$ –dimensionless lattice spacing, and the relative coordinates of the equilibrium positions of the atoms in the lattice.

Here m_1 is the mass of the particle; m_2 is the mass of an atom in the crystal; E_0 is the initial energy of the particle; σ and ε are the parameters of the Lennard-Jones potential; $\varkappa$ is the stiffness of the bond of the harmonic oscillator (determined from the characteristic temperature of the solid).

Since, in practice, of interest are the values of the energy accommodation coefficient $\alpha = 1 - E_f/E_0$ (E_f is the energy of the reflected particle) not for an individual particle with its impact parameters $\bar{x}_c, \bar{y}_c$, but the mean value–

for a large ensemble of incident particles, it is necessary to average the individual values of α over the range of values $\bar{x}_c, \bar{y}_c$ (and in some cases also over ψ). In passing to a polycrystal the averaging must also be carried out over φ.

3. Integration of the equations of motion of the particles participating in the energy exchange was carried out on a BESM-2M computer by the Runge–Kutta method with a variable integration step. The accuracy of the computation was checked by the total energy of the system, which remained constant to a prescribed degree of accuracy. In the calculations the semi-infinite crystal was replaced by a finite block of atoms consisting of the nearest neighbors of the target atom up to the 7th order inclusive (59 atoms in all). To estimate the error introduced by this assumption, a calculation was performed for the case $\bar{m} = 0.5$; $\bar{w} = 1$; $\bar{\varepsilon} = 0.01$; $\varphi = 0$; $\bar{d} = 1$; $x_c = y_c = 0$, with a block containing different numbers of atoms. The following results were obtained:

α	Order of neighbors included	4	5	6	7
α	p. c.	0.89667	0.89709	0.89723	0.89728
α	f. c. c.	0.88765	0.89032	0.89056	0.89087
α	b. c. c.	0.90131	0.90161	0.90187	0.90216

Thus, the indicated choice of block provides 3-4 correct significant figures in the energy accommodation coefficient. The interaction of the incident particle with the crystal was restricted to a layer above the surface of thickness 3σ. The error introduced by this did not exceed that described above.

For averaging α over all possible (with allowance for symmetry) values of $\bar{x}_c$ and $\bar{y}_c$, the Gaussian quadrature formula was used. For a simple cubic lattice and for the values of the dimensionless parameters given above, the following dependence of α_{av} on the number of trajectories N, and hence on the highest degree of the approximating polynomial n, was obtained:

N	1	3	6	10
n	3	7	11	15
α_{av}	0.80499	0.69745	0.80095	0.78860

The largest changes in α for individual trajectories occur on the diagonal of the elementary cube. The dependence shown in Fig. 1 indicates that a satisfactory approximation of it can be achieved by a polynomial of no lower than the 10th degree; consequently, the minimum number of calculated trajectories required for averaging is 6. The coincidence of α_{av} for $N = 1$ and 6 should be regarded as accidental. From the data given above it is seen that in the scheme adopted below, with averaging over 6 trajectories, α_{av} was determined with an accuracy of ~ 0.01.

In Ref. ([1]) calculations were made of the accommodation coefficient at low energies of an incident particle falling on a two-layer block of 200 atoms at an angle $\varphi = \pi/4$ in the direction of the diagonal of the surface face. Averaging was performed over target points uniformly distributed over the surface. For comparison we give the results of Ref. ([1]) and those specially calculated by the proposed method for the same case:

p. c.; $\bar{m} = 0.5$; $\bar{w} = 0.08$; $\bar{\varepsilon} = 0.00192$; $\bar{d} = 0.8$; $\varphi = \psi = \pi/4$.

	Work ([1])	Work ([1])	Work ([1])	Work ([1])	Work ([1])	Our method
N	2	8	18	32	72	21
n	1	3	5	7	11	11
α_{av}	0.030	0.140	0.136	0.134	0.139	0.1411

4. Calculations were carried out demonstrating the dependence of the energy accommodation coefficient on the type of lattice, $\bar{d}$, $\bar{m}$, $\bar{w}$. The range of $\bar{w}$ considered corresponds to velocities $\sim 10 \div 20$ km/sec.

$$\bar{m} = 0.5; \qquad \bar{w} = 1; \qquad \bar{\varepsilon} = 0.01; \qquad \varphi = 0$$

α_{av}	Lattice type	$\bar{d} = 0.65$	$\bar{d} = 0.8$	$\bar{d} = 1.0$	$\bar{d} = 1.2$
α_{av}	s.c.	0.7147	0.7554	0.8009	–
α_{av}	f.c.c.	–	0.6692	0.7422	0.7706
α_{av}	b.c.c.	–	0.7576	0.7975	0.8266

b.c.c. $\bar{w} = 1$; $\bar{\varepsilon} = 0.01$; $\bar{d} = 0.8$; $\varphi = 0$

	$\bar{m}=0.25$	$\bar{m}=0.50$	$\bar{m}=0.75$
$4\bar{m}/(\bar{m}+1)^2$	0.6400	0.8889	0.9855
α_{av}	0.5190	0.7576	0.8816

b.c.c. $\bar{m}=0.5$; $\bar{\varepsilon}=0.01$; $\bar{d}=0.8$; $\varphi=0$

	$\bar{w}=0.7$	$\bar{w}=1.0$	$\bar{w}=1.4$
α_{av}	0.7713	0.7576	0.7554

The proposed method for investigating interaction processes can be generalized to estimate the influence of adsorbate, surface reactions, and lattice defects on energy exchange in a rarefied flow, and also makes it possible to obtain the characteristics of the transfer of tangential and normal momenta. The results of the calculations may serve as a guide in evaluating experimental data obtained when the surface conditions have not been strictly identified.

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REFERENCES

1. R. Oman, A. Bogan et al., *Am. Inst. Aeronaut. and Astron. J.*, **2**, 10 (1964).

Note: Figure translations are in progress. See original paper for figures.