# CAPTURE OF GAS ATOMS ON A SOLID SURFACE

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Capture of gas particles is usually considered under the assumption that collisions with surface atoms occur against a background of one-dimensional steady-state potential attraction, due to collective interaction effects. If the direct reflection from a solid wall is independent of the presence of a surface potential, then the total scattering function can easily be expressed as a function of the scattering with the field absent [1].

Capture occurs if the gas particle energy, following collision with the surface atoms, is less than the depth of the potential well $E_D$. Following from the one-dimensional nature of the attractive potential, the possibility of capture is determined only by the particle energy along the normal $E_\perp = E\cos^2\theta_{rD}$, where $\theta_{rD}$ is the angle of reflection from a surface element. If $E_\perp < E_D < E$, the particle is called a skip particle or a semicaptured particle. Such particles are reflected from the potential barrier and experience multiple collisions with the body surface.

When one calculates capture probability one usually ignores the difference between captured and skip atoms. In particular, it is conventional to consider that these and other atoms fly out from the attractive zone in accordance with the diffusion law at the surface temperature.

However, it should be noted that omitting the effect of semicaptured atoms from the calculation in theoretical models can lead to a contradiction with experimental data for large energies of the incident flow and high angles of incidence. This contradiction manifests itself particularly clearly in the rather wide distribution obtained from cube theory [2]. If tangential momentum is conserved in collision of a gas particle with an oscillating smooth cube the result is that the capture probability depends only on $E_\perp = E_i\cos^2\theta_i$, where $\theta_i$ is the angle of incidence. In other words, for arbitrary large energy $E_i$ of the incident flow one finds an angle of incidence $\theta_i$ where all the gas particles will be captured with an overwhelming probability (the effect of particle energy becomes arbitrarily small. This result, which does not make sense from the physical viewpoint, is not confirmed by experimental data, which indicates that the capture coefficient $P_t$ does not exceed 30-50% as a function of the angle of incidence, and for large energies there are no captures for any value $\theta_i$ [3, 4].

If one models the surface as a mass of nonrelated harmonic oscillators, oscillating along the normal, one finds the following expression for the capture probability [3]:

$$P_t = \frac{1}{2}\left\{1 + \operatorname{erf}\left[\frac{1+\mu}{2\mu^{1/2}}\left(\frac{E_D}{kT_S}\right)^{1/2}\left(1 - \frac{1-\mu}{1+\mu}\left(1 + \frac{E_i\cos^2\theta_i}{E_D}\right)^{1/2}\right)\right]\right\}, \quad (1)$$

where $\mu = m_a/m_S$, $m_a$, $m_S$ are the masses of the gas and surface atoms; and $T_S$ is the surface temperature.

A comparison of the experimental data of [3] on scattering of potassium atoms by a semicrystalline tungsten surface with the result of the cube theory, as in Fig. 1, shows that the capture probability is described satisfactorily by Eq. (1) only for small incidence angle of the atomic beam. The measured results of [3] are shown in Fig. 1 by points 1' for $\theta_i = 16.5°$ and by 4' for $\theta_i = 75°$, and the cube model data, Eq. (1), are illustrated by curves 1"–4" for incidence angles 16.5; 45; 60; 75°, respectively.

A generalization of cube theory, to allow for loss of tangential momentum in collisions between the gas and the surface, was proposed in [5], where the surface was built up of partially shaded spherical spheres. In [4] capture was studied under the assumption that the adsorbed atom interacts with a diatomic molecular surface.

In this paper the non-one-dimensional interaction is taken into account by modeling the body surface with a random field with some fluctuation in slope. It takes into account the following factors: 1) large-scale roughness; 2) atomic-scale roughness; 3) the effect of skip atoms.

One must describe the surface statistically because of the three-dimensional structure of the crystalline lattice and the temperature fluctuations of the solid surface atoms. According to an estimate in [3], the

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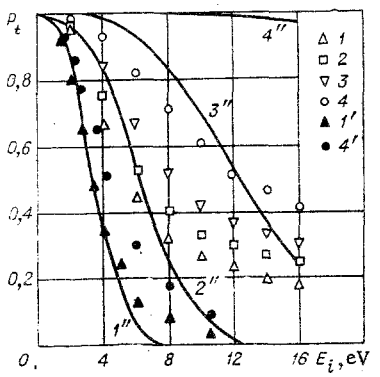


Fig. 1

average amplitude of thermal oscillations is 0.6 Å, which is quite comparable with the radius of the tungsten atom ($R_W \simeq 1.35$ Å). For actual surfaces a typical roughness has dimensions which are appreciably greater than the interatomic distances in the solid, and the large-scale statistical nonuniformity may serve to simulate the polycrystalline surface structure.

We shall consider first the case where the nonuniformities are much larger than the constant of a crystalline lattice. We assume that the cube model is valid only locally, i.e., for reflection of atoms from a part of the surface small compared with the size of the nonuniformity. The direction of the collective attraction forces acting on the incident gas atom and of repulsion from the oscillatory cube is determined by the local normal to the surface. As a specific example of surface roughness we choose a random field created with the help of spectral decomposition [6].

Typical results of calculations performed by the direct numerical modeling method of [6, 7] are shown in Fig. 1, and compared with cube theory and the measured data of [3]. The capture probability $P_t$ was calculated as the average of 10,000 trials (the numerical results in Fig. 1 are denoted by points 1-4 for incidence angle 16.5; 45; 60; 75°, respectively). The depth of the potential well $E_D = 2.3$ eV, the mass ratio $\mu = 0.21$, and the body temperature $T_S = 1200$°K correspond to scattering of potassium atoms at a tungsten surface under the experimental conditions of [3]. The roughness slope is a free parameter in the model considered. The calculated data in Fig. 1 were obtained for $\sigma = \langle \mathrm{tg}^2\varphi \rangle^{1/2} = 1$, where $\varphi$ is the random slope angle of the surface element. The presence of large-scale fluctuations considerably alters the angular dependence of the capture coefficient. However, the model assumed for interaction describes the behavior of $p_t$ with respect to energy only qualitatively, and needs further refinement. The roughness increases the encounter angle of the incident atom with the surface element in the case of normal incidence, and decreases it for glancing trajectories. Here the capture probability for fast particles remains unrealistically high. One cannot bring $P_t$ close to the experimental data in the region of high atomic beam energies $E_i$ by varying $\sigma$.

The numerical investigations have shown that the above nature of the dependence of capture coefficient on $\theta_i$ and $E_i$ is retained even when one allows for roughness at the atomic level. One of the causes for $P_t$ being overestimated is the incorrect assumption that the capture event in terms of energy occurs in the direction of the force field, without allowance being made for skip atoms.

In order to estimate the effect of semicapture and atomic-scale roughness we assume the following interaction scheme. The solid surface is built up as a two-dimensional random function. The attractive field, modeled by a rectangular potential well, will be considered as acting in a direction normal to the average surface level. The incident flow atom, reaching a part of the surface with a local normal n, collides with a surface atom. The collision is postulated to be smooth, and the change in momentum occurs in the direction n

$$v_{1n} = \frac{2u_{0n}}{\mu + 1} + \frac{\mu - 1}{\mu + 1} v_{0n},$$

where $v_{0n}$, $v_{1n}$ are the velocity components of the gas particle along the local normal, before and after the collision; and $u_{0n}$ is the random velocity of the surface atom with dispersion $(kT_S/m_S)^{1/2}$, describing thermal oscillations at temperature $T_S$. We note that after reflection from the surface element, the gas atom may experience repeated collisions with the surface before departing over the boundary of the force field.

A particle is regarded as captured if its total energy $E < E_D$, and as semicaptures if $E_\perp < E_D < E$, where $E_\perp = E\cos^2\theta_{rD}$ and $\theta_{rD}$ is the angle of reflection from the surface element. The trajectories of the semicaptured atoms are tracked until they transfer to the class of captured or scattered particles. The surface is modeled as plane tetragons with random slope [7].

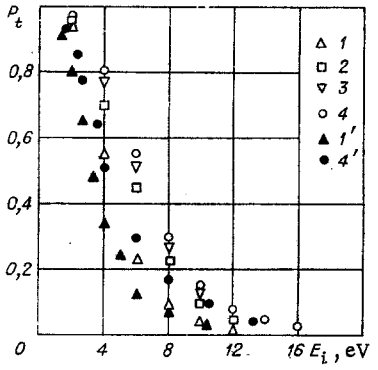


Fig. 2

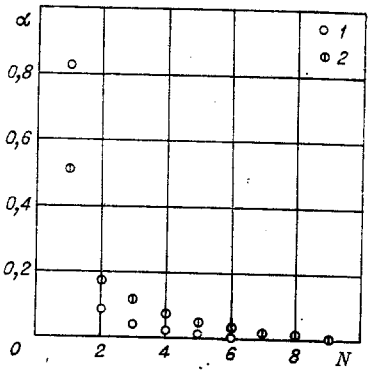


Fig. 3

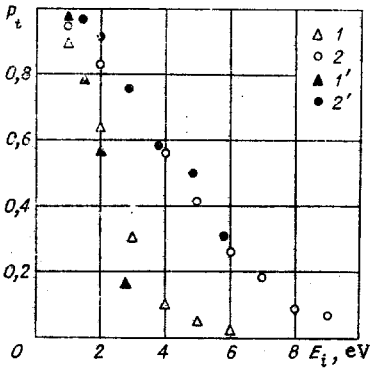


Fig. 4

Figure 2 shows the capture probability for K atoms on a W surface, computed for $\sigma = 0.2$ (the notation is the same as in Fig. 1). The relative number of atoms $\alpha$, leaving the attraction zone after N-fold reflection from the potential barrier is shown in Fig. 3 ($1 - \theta_i = 75°$, $E_i = 4$ eV, $2 - \theta_i = 75°$, $E_i = 12$ eV). The lack of agreement with experimental data in the high-energy region is eliminated by taking account of skip atoms, which have a high escape probability because of the fluctuations in the velocity vector direction. Even for an energy of $E_i \sim E_D$ the fraction of semicaptured atoms is substantial; e.g., for an inclined incidence of a high-energy beam with $E_i \gg E_D$ about 40% of the scattered atoms experience multiple collisions with the surface, without exiting from the attractive field. Semicapture followed by ejection is not accompanied by relaxation of the translation energy of the atom, since the time spent by an atom in the semicaptured state (according to the data of Fig. 3) exceeds the collision time with an individual lattice atom by no more than an order of magnitude, and is estimated to be $10^{-14}$-$10^{-13}$ sec. The lifetime of a fully captured atom measured in [3] was $10^{-4}$ sec.

Figure 4 shows the numerical results for scattering of sodium atoms on a tungsten surface ($\mu = 0.125$, $\sigma = 0.2$, and points 1 and 2 correspond to incidence angles of 10 and 70°). The experimental data of [4] for capture of Na on a W surface (110) for the same incidence angles are indicated by points 1' and 2'. By analyzing the experiments in [4] we obtain the value for the depth of the potential well $E_D = 2.6$ eV, which was used in the calculations.

When Na and K atoms are reflected from a tungsten surface they experience complete ionization, associated with the comparatively large value of the attraction potential. A considerable difference was noted in [4] in the capture probability for scattering on a semicrystalline surface and on a monocrystal. The model used allows us to describe the experimental results using a chosen parameter $\sigma$, describing the surface structure.

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# RELATIVISTIC ELECTRON BEAM WITH A VARIABLE DEGREE OF CHARGE NEUTRALIZATION

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A rather large number of theoretical papers have appeared on the steady states of relativistic beams which are uniform along the axis (cf. reviews [1, 2]), but under actual experimental conditions the degree of charge neutralization of a beam may vary considerably along the tube axis. In quasistationary and stationary systems the ion density may vary appreciably along the length when there are longitudinal sinks [3]. In addition, a number of papers (e.g., [4]) consider the focusing of beams in a guide tube by a pressure gradient along the beam. Thus, it is interesting to consider the equilibrium state of a beam for a variable degree of charge neutralization along the tube through which a quasisteady beam is propagated.

We assume that a beam with a current I is injected along the axis of a metal tube of length 2L with a density of neutral particles $n_0(z)$. The ion density $n_i(z)$ arising as a result of ionization will also vary. For simplicity we assume that the beam is narrow enough so that we can consider $n_0$, $n_i$, and $n_e$, independent of the radius $\rho$. We denote the characteristic scale of the nonuniformity of the $n_i$ distribution by $l$, where $l \lesssim L$.

We assume that the density of neutral atoms, and consequently the ion density, is maximum at $z = 0$ ($-L \leq z \leq L$). By assumption the state of the beam varies from nearly forcefree at the ends of the tube toward quasineutral, but the conditions for quasineutrality and force-free motion are not satisfied exactly ($n_e > n_i \gtrsim n_e/\gamma^2$, where $\gamma$ is the ratio of the total energy of an electron to its rest energy). Under these conditions it is required to find the characteristics of an axially symmetric beam ($n_e(z)$, $n_i(z)$, and $\gamma(z)$), taking account of the effect of self-fields on the motion of beam particles.

If $\mathbf{v}$ if the velocity of an electron, and $\mathbf{E}$ and H are the intensities of the electric and magnetic fields, the equation of motion of an electron can be written in the form

$$\dot{\mathbf{v}} = -\frac{e}{m\gamma}\left\{\mathbf{E} - \frac{1}{c^2}\mathbf{v}(\mathbf{vE}) + \frac{1}{c^2}[\mathbf{vH}]\right\}, \tag{1}$$

where e and m are the charge and mass of the electron, and c is the velocity of light.

We use the adiabatic approximation to solve (1); i.e., we assume that $\mathbf{E}$, H, and $\gamma$ vary slowly along the axis of the tube. Then we can set $E_z \approx 0$.

The projection of (1) along the direction of the radius $\rho$ of a cylindrical coordinate system gives

$$\ddot{\rho} + \frac{e}{m\gamma}\left\{E_\rho\left(1 - \frac{\dot{\rho}^2}{c^2}\right) - \frac{\dot{z}}{c}H_\theta\right\} = 0. \tag{2}$$

The field components $E_\rho$ and $H_\theta$ are $E_\rho = 2\pi e\rho(n_i - n_e)$ and $H_\theta = -2\pi e\rho n_e\beta_z$, where $n_e(z)$ is the electron density in the beam, $\beta_z = v_z/c$, and $v_z$ is the average longitudinal velocity of the electrons. Then (2) can be written in the form

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