EFFECT OF ROUGHNESS ON THE INTERACTION BETWEEN LOW-DENSITY GAS AND THE SURFACE OF A SOLID

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The effect of roughness on the reflection of molecules of a low-density gas from the surface of a solid is studied. An expression is derived for the transform for a single reflection from a homogeneous roughness which permits simple programming for a computer. A simple approximation to this expression is considered which is applicable over a broad range of roughness parameters and of gas-molecule angles of incidence. Based on this approximation, the angular distributions of reflected molecules are calculated and a comparison is made with similar distributions taken from [1].

The result of an interaction between molecules of a low-density gas and the surface of a solid for a given incident velocity $\mathbf{u}_1$ is characterized by a molecular density distribution F with respect to the reflected velocities $\mathbf{u}_2$ (Fig. 1). Because of the roughness, reflection of molecules from the surface may occur after one, two, or more collisions with microprojections. The quantity F is therefore conveniently represented in the form [1]

$$F = \sum_{n=1}^{\infty} F_n$$

where F_n is the density distribution for molecules reflected after n-fold collisions with microprojections (transform for n-fold reflections). Ordinarily, it is sufficient to know only the first term F_1 of this series since molecules undergoing more than one collision adapt practically completely to surface conditions.

The problem of the effect of roughness on the structure of F_1 (for a known law F_0 for the reflection of molecules from an ideally smooth surface) has been discussed in the literature mainly in a simplified form where the roughness was assumed slight (small slope variance σ_t^2) and isotropic, and the reflection law F_0 was assumed specular. A more complete study of the structure of F_1 was given in [1], where the general problem of reflection from a homogeneous isotropic surface was discussed and a simple approximation was proposed for the case of normal slight roughness ($\sigma_t \lesssim 0.3$) and angles of incidence θ_1 not close to 90°. The asymptote of F_1 for $\theta_1 \to 90°$ and $\sigma_t \to 0$ was discussed in [2]. In other cases, however, the solution obtained in [1] is in extremely cumbersome form and hardly suitable for numerical calculations. In addition, it fails to take the anisotropy of real surfaces into account.

In order to obtain a more convenient general expression for F_1 which would also take into account surface anisotropy, we consider the following method for determination of the desired transform.

Let a gas molecule undergo a single interaction with the surface of a solid; i.e., the following events occur (Fig. 1): A) free flight of a molecule at a velocity $\mathbf{u}_1$ along the ray MO from infinity to some point O; B) interaction with the surface in the neighborhood of point O; C) the surface in the neighborhood of point O is oriented with its normal within the elementary solid angle $d\omega_0 = \sin\theta_0 d\theta_0 d\varphi_0$; D) reflection from the surface at a velocity $\mathbf{u}_2$ in the interval $d\mathbf{u}_2$; E) free flight along the ray ON from the point O to infinity.

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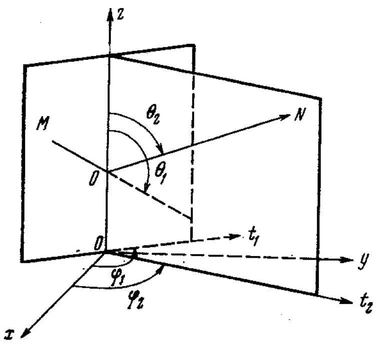

Fig. 1

The desired transform is then found from the expression [1]

$$F_1 du_2 = \int\limits_{z_0=-\infty}^{z_0=\infty} \iint\limits_{\varphi_0\,\theta_0} p(ABCDE) \tag{1}$$

where p(ABCDE) is the probability of the product of the events mentioned above. The limits of integration with respect to the angles φ_0 and θ_0 are determined by the initial conditions and depend on the angles φ_1, φ_2, θ_1, and θ_2. In the approximation [1], they were assumed to be, respectively, $(0, 2\pi)$ and $(\pi/2, \pi)$ for simplicity, but this limited the region of applicability of the approximation to the angles $\theta_1 \gtrsim 105°$. Exact values of the limits can be found from geometric consideration of the problem, which leads after a number of transformations to the following result:

$$\iint\limits_{\varphi_0\,\theta_0} = \sum_{i=1}^{3} \int\limits_{\varphi_H^i}^{\varphi_b^i} \int\limits_{\theta_H^i}^{\theta_b^i} \tag{2}$$

where

$$\varphi_H^1 = \varphi_b^3 - 2\pi = \begin{cases} \varphi_1 + \operatorname{arc\,tg}\left[\dfrac{\operatorname{ctg}\theta_2}{\sin(\varphi_2-\varphi_1)\operatorname{ctg}\theta_1} - \operatorname{ctg}(\varphi_2-\varphi_1)\right] & \text{for} \quad \varphi_2 > \varphi_1 \\ \varphi_2 - \pi + \operatorname{arc\,tg}\left[\dfrac{\operatorname{ctg}\theta_1}{\sin(\varphi_1-\varphi_2)\operatorname{ctg}\theta_2} - \operatorname{ctg}(\varphi_1-\varphi_2)\right] & \text{for} \quad \varphi_2 < \varphi_1 \end{cases}$$

$$\varphi_H^2 = \varphi_b^1 = \begin{cases} \varphi_1 + \pi/2 & \text{for} \quad \varphi_2 > \varphi_1 \\ \varphi_2 - \pi/2 & \text{for} \quad \varphi_2 < \varphi_1 \end{cases},$$

$$\varphi_H^3 = \varphi_b^2 = \begin{cases} \varphi_2 + \pi/2 & \text{for} \quad \varphi_2 > \varphi_1 \\ \varphi_1 - \pi/2 & \text{for} \quad \varphi_2 < \varphi_1 \end{cases}$$

$$\theta_H^1 = \theta_H^2 = \theta_H^3 = 0$$

$$\theta_b^1 = \begin{cases} -\operatorname{arc\,tg}\left[\dfrac{\operatorname{ctg}\theta_1}{\cos(\varphi_0-\varphi_1)}\right] & \text{for} \quad \varphi_2 > \varphi_1 \\ -\operatorname{arc\,tg}\left[\dfrac{\operatorname{ctg}\theta_2}{\cos(\varphi_0-\varphi_2)}\right] & \text{for} \quad \varphi_2 < \varphi_1 \end{cases}, \qquad \theta_b^2 = \frac{\pi}{2}$$

θ_b^3 is determined by the expression for θ_b^1 with replacement of the condition $\varphi_2 > \varphi_1$ by $\varphi_2 < \varphi_1$ and vice versa.

We now consider the function inside the integral sign in Eq. (1), assuming that the original surface is a three-dimensional, anisotropic, differentiable random field $\xi(x, y)$. This function can be represented in the form

$$p(ABCDE) = p(A)\, p(E \mid A)\, p(B \mid AE)\, p(C \mid AEB)\, p(D \mid AEBC) \tag{3}$$

where $p(\mu \mid \nu)$ is the conditional probability for event μ under the condition event ν has occurred. Following [1], we cut the surface by a dihedral angle having the vertex 0z and faces that pass through the rays MO and ON. The stochastic function

$$\xi(t) = \begin{cases} \xi(t\cos\varphi_1, t\sin\varphi_1) & \text{for} \quad t < 0 \\ \xi(t\cos\varphi_2, t\sin\varphi_2) & \text{for} \quad t > 0 \end{cases} \tag{4}$$

is then formed in the section.

Let $f(t)$ be a specified curve. We then introduce another function

$$\delta(t) = \begin{cases} 1, & \text{if} \quad \xi(t) > f(t) \\ 0, & \text{if} \quad \xi(t) < f(t) \end{cases} \tag{5}$$

and denote by $S(t_1, t_2)$ an event where the function $\delta(t) = 0$ in the interval (t_1, t_2); $p_n(t_1, t_2)$ is the probability that the function $\delta(t)$, being in the zero state at the time t_1, changes its state n times by the time t_2. Using this notation, one can write

$$p_0(t_1, t+\Delta t) = p_0(t_1, t) - p_0(t_1, t)\sum_{n=1}^{\infty} p_n[t, t+\Delta t \mid S(t_1, t)] \tag{6}$$

Since the function $\xi(t)$ is differentiable, the function $\delta(t)$ will be ordinary and in the small interval Δt

$$\begin{aligned}\sum_{n=1}^{\infty} p_n[t, t+\Delta t \mid S(t_1, t)] &= p_1[t, t+\Delta t \mid S(t_1, t)] + 0(\Delta t) = \\ &= d[t \mid S(t_1, t)]\,\Delta t + 0(\Delta t)\end{aligned} \tag{7}$$

where $d[t \mid S(t_1, t)]$ is the conditional probability density for an excursion of $\xi(t)$ through $f(t)$ at the time t for the condition $S(t_1, t)$. Substituting Eq. (7) into Eq. (6), we have

$$\frac{p_0(t_1, t+\Delta t) - p_0(t_1, t)}{\Delta t} = -p_0(t_1, t)\{d[t \mid S(t_1, t)] + 0(1)\}$$

Letting $\Delta t \to 0$, we obtain a differential equation from which we find

$$p_0(t_1, t_2) = \exp\left\{-\int_{t_1}^{t_2} d[t \mid S(t_1, t)]\,dt\right\} \tag{8}$$

In particular, if $\xi(t)$ is a Poisson process, $d[t \mid S(t_1, t)] = d(t)$, and Eq. (8) takes the form

$$p_0(t_1, t_2) = \exp\left[-\int_{t_1}^{t_2} d(t)\,dt\right]$$

In the general case [3]

$$d[t \mid S(t_1, t)] = \int_{\dot f(t)}^{\infty} \rho[f(t), \dot\xi(t) \mid S(t_1, t)]\,[\dot\xi(t) - \dot f(t)]\,d\dot\xi(t) \tag{9}$$

where the dots indicate differentiation with respect to t, and $\rho[f(t), \xi(t) \mid S(t_1, t)]$ is the conditional density of the joint distribution of $\xi(t)$ and $\dot\xi(t)$ for the value $\xi(t) = f(t)$ and the condition $S(t_1, t)$.

We now assume that the function $f(t)$ describes the trajectory of a gas molecule, i.e.,

$$f(t) = \xi(0) + \begin{cases} t\,\mathrm{ctg}\,\theta_1 & \text{for} \quad t < 0 \\ t\,\mathrm{ctg}\,\theta_2 & \text{for} \quad t > 0 \end{cases} \tag{10}$$

Considering Eqs. (8)-(10), we then obtain

$$p(A) = \exp\left\{-\int_{-\infty}^{0}\int_{\mathrm{ctg}\,\theta_1}^{\infty} \rho[f(t), \dot\xi(t) \mid S(-\infty, t)]\,[\dot\xi(t) - \mathrm{ctg}\,\theta_1]\,d\dot\xi(t)\,dt\right\} \tag{11}$$

$$p(E \mid A) = \exp\left\{-\int_{0}^{\infty}\int_{\mathrm{ctg}\,\theta_2}^{\infty} \rho[f(t), \dot\xi(t) \mid S(-\infty, 0), S(0, t)]\,[\dot\xi(t) - \mathrm{ctg}\,\theta_2]\,d\dot\xi(t)\,dt\right\} \tag{12}$$

$$p(B \mid AE) = \int_{\mathrm{ctg}\,\theta_1}^{\infty} \rho[f(0), \dot\xi(0) \mid S(-\infty, 0), S(0, \infty)]\,[\dot\xi(0) - \mathrm{ctg}\,\theta_1]\,d\dot\xi(0) \tag{13}$$

We next consider the probability $p(C \mid AEB)$. It is

$$\begin{aligned}p(C \mid AEB) = &\left\{\int_{\xi_x(0)}\int_{\xi_y(0)} \rho[\xi_x(0), \xi_y(0) \mid S(-\infty, 0), S(0, \infty), \xi(0)]\,d\xi_x(0)\,d\xi_y(0)\right\}^{-1} \times \\ &\times \rho[\xi_x(0), \xi_y(0) \mid S(-\infty, 0), S(0, \infty), \xi(0)]\,d\xi_x(0)\,d\xi_y(0)\end{aligned}$$

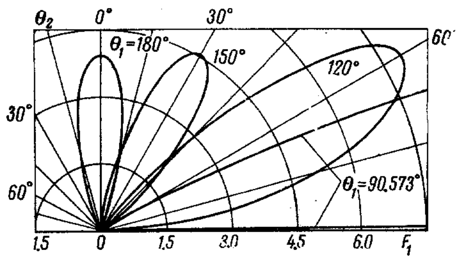

Fig. 2

where

$$\xi_x(0) = \frac{\partial \xi(x, y)}{\partial x}\bigg|_{x=y=0}, \quad \xi_y(0) = \frac{\partial \xi(x, y)}{\partial y}\bigg|_{x=y=0}$$

Transforming to the spherical coordinates θ_0 and φ_0 and remembering

$$\xi_x(0) = -\operatorname{tg}\theta_0 \cos\varphi_0, \quad \xi_y(0) = -\operatorname{tg}\theta_0 \sin\varphi_0$$

we obtain

$$p(C \mid AEB) = \left\{\int\limits_{\varphi_0}\int\limits_{\theta_0} \rho\,[\xi_x(0), \xi_y(0) \mid S(-\infty, 0), S(0, \infty), \xi(0)]\,\frac{\sin\theta_0}{\cos^3\theta_0}\,d\theta_0\,d\varphi_0\right\}^{-1} \times$$
$$\times \rho\,[\xi_x(0), \xi_y(0) \mid S(-\infty, 0), S(0, \infty), \xi(0)]\,\frac{\sin\theta_0}{\cos^3\theta_0}\,d\theta_0\,d\varphi_0 \tag{14}$$

The region of integration for the angles θ_0 and φ_0 in this equation agrees with that in Eq. (2). If the function ξ(x, y) is normal,

$$\rho\,[\xi_x(0), \xi_y(0) \mid S(-\infty, 0), S(0, \infty), \xi(0)] = \rho\,[\xi_x(0) \mid S(-\infty, 0), S(0, \infty)]\,\rho\,[\xi_y(0) \mid S(-\infty, 0), S(0, \infty)] \tag{15}$$

and Eq. (14) is correspondingly simplified.

Finally, the last factor in Eq. (3), the probability p(D | AEBC), has the form

$$p(D \mid AEBC) = F_0 d\mathbf{u}_2 = F_0 u_2^2\,du_2 \sin\theta_2 d\theta_2\,d\varphi_2 \tag{16}$$

where the reflection law F_0 is assumed known.

Equations (1)-(4) and (10)-(16) completely define the transform F_1; however, it is still unsuitable for numerical calculations. The main difficulty is in the calculation of integrals such as

$$I = \int\limits_{\dot f(t)}^{\infty} \rho\,[f(t), \dot\xi(t) \mid S(T)][\dot\xi(t) - \dot f(t)]\,d\dot\xi(t) \tag{17}$$

where T is some interval preceding or following the time t. We use the following approximation to evaluate such integrals. First, we limit the magnitude of T to the correlation interval T_k. This is permissible because by definition [4] any two sections of the stochastic function ξ(t) separated by an interval $T > T_k$ can be considered independent of one another. Second, we replace S(T) by the condition $\xi(t) < f(t)$ at a finite number of points $t_i \in T$, i = 1, ..., n. Without concerning ourselves about the optimal choice of these points, we shall assume they are equidistant from one another, with the first point coinciding with the beginning of the interval T and the last point coinciding with the end of the interval. The integral (17) is then written in the form

$$I \approx \int\limits_{\dot f(t)}^{\infty} \rho\,[f(t), \dot\xi(t) \mid S(t_i, i = 1 \div n)][\dot\xi(t) - \dot f(t)]\,d\dot\xi(t) =$$
$$= \left\{\int\limits_{-\infty}^{f(t_1)} \cdots \int\limits_{-\infty}^{f(t_n)} \rho\,[\xi(t_1), \ldots, \xi(t_n)]\,d\xi(t_n) \ldots d\xi(t_1)\right\}^{-1} \int\limits_{\dot f(t)}^{\infty}\int\limits_{-\infty}^{f(t_1)} \cdots$$
$$\cdots \int\limits_{-\infty}^{f(t_n)} \rho\,[f(t), \dot\xi(t), \xi(t_1), \ldots, \xi(t_n)][\dot\xi(t) - \dot f(t)]\,d\xi(t_n) \ldots d\xi(t_1)\,d\dot\xi(t) \tag{18}$$
$$t_i = t_1 - T(i-1)/(n-1), \quad T \leqslant T_k, \quad i = 1 \div n$$

By making the number n sufficiently large, the error resulting from the replacement of Eq. (17) by Eq. (18) can be reduced to practically zero. Trial calculations indicate that the number n for actual surfaces ordinarily is no greater than 10 for a relative error of 10%. The case n = 1, where the condition $S(t_i$, i = 1, ..., n) reduces to $S(t_1)$, is of particular interest. Remembering that the time t_1 directly precedes or follows the time t, we then have

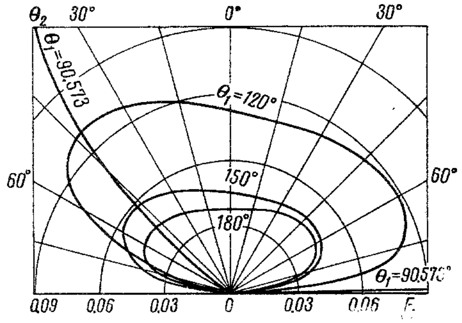

Fig. 3

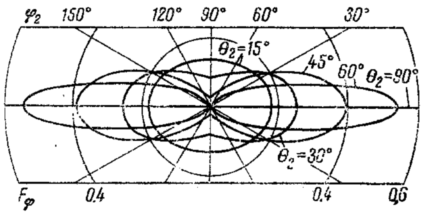

Fig. 4

$$I = \lim_{t_1' \to t} \left\{ \int_{-\infty}^{f(t_1')} \rho\,[\xi(t_1')]\, d\xi(t_1') \right\}^{-1} \int_{f(t)}^{\infty} \int_{-\infty}^{f(t_1')} \rho\,[f(t), \dot{\xi}(t), \xi(t_1')]$$

$$d\xi(t_1')\, d\dot{\xi}(t) = \lim_{t_1' \to t} \rho\,[f(t)] \left\{ \int_{-\infty}^{f(t_1')} \rho\,[\xi(t_1')]\, d\xi(t_1') \right\}^{-1} \times$$

$$\times \int_{f(t)}^{\infty} \int_{-\infty}^{f(t_1')} \rho\,[\xi(t_1') \mid f(t)]\, \rho\,[\dot{\xi}(t) \mid f(t), \xi(t_1')]\, d\xi(t_1')\, d\dot{\xi}(t)$$

The conditional density $\rho[\xi(t_1') \mid f(t)]$ converts into the δ-function $\delta[\xi(t)-f(t)]$ for $t_1' \to t$, and Eq. (18) takes the form

$$I = \rho\,[f(t)] \left\{ \int_{-\infty}^{f(t)} \rho\,[\xi(t)]\, d\xi(t) \right\}^{-1} \int_{\dot{f}(t)}^{\infty} \rho\,[\dot{\xi}(t) \mid f(t)]\, d\dot{\xi}(t) \tag{19}$$

If the function $\xi(t)$ is normal, $\rho[\dot{\xi}(t) \mid f(t)] = \rho[\dot{\xi}(t)]$ and Eq. (19) is correspondingly simplified. Taking Eqs. (1), (3), (11)-(17), and (19) into account, it is easy to obtain the following expression for the desired transform:

$$F_1 = \frac{1}{\pi \sigma_x \sigma_y} \left\{ 1 - \frac{1}{\alpha_1} \sqrt{\frac{2}{\pi}}\, [1 - \Phi(\alpha_1)]^{-1} \exp\left(-\frac{\alpha_1^2}{2}\right) \right\} \times$$

$$\times \left\{ \Phi(\alpha_2) - \Phi(\alpha_1) + \sqrt{\frac{2}{\pi}} \left[\frac{1}{\alpha_2} \exp\left(-\frac{\alpha_2^2}{2}\right) - \frac{1}{\alpha_1} \exp\left(-\frac{\alpha_1^2}{2}\right) \right] \right\}^{-1} \times$$
$$\times \int_{\varphi_0} \int_{\theta_0} F_0 \frac{\sin\theta_0}{\cos^3\theta_0} \exp\left[-\frac{\mathrm{tg}^2\,\theta_0}{2} \left(\frac{\cos^2\varphi_0}{\sigma_x^2} + \frac{\sin^2\varphi_0}{\sigma_y^2} \right) \right] d\theta_0\, d\varphi_0 \tag{20}$$

where

$$\alpha_1 = \frac{\mathrm{ctg}\,\theta_1}{\sigma_{t1}}, \quad \alpha_2 = \frac{\mathrm{ctg}\,\theta_2}{\sigma_{t2}}, \quad \Phi(\alpha) = \frac{2}{\sqrt{2\pi}} \int_0^{\alpha} \exp\left(-\frac{t^2}{2}\right) dt$$

and σ_x^2, σ_y^2, $\sigma_{t_1}^2$, and $\sigma_{t_2}^2$ are the variances of the slopes [i.e., the variances of the derivative $\dot{\xi}(t)$] along the x and y axes and in the direction of the flight of a molecule before and after collision with the surface. Note that if the x and y axes coincide with the principal directions of the roughness, the variance of the slopes in an arbitrary direction t is expressed through the variances σ_x^2 and σ_y^2 by the relation [5]

$$\sigma_t^2 = \sigma_x^2 \cos^2\psi + \sigma_y^2 \sin^2\psi \tag{21}$$

where ψ is the angle between the direction t and the x axis.

Thus the desired transform is completely determined by assignment of the variances σ_x^2 and σ_y^2 and by the initial angles of incidence φ_1 and θ_1.

The approximation (19), (20) is applicable in those cases where the trajectory of the molecule satisfies one of the two conditions:

1) $|\dot{f}(t)/\sigma_t| \gtrsim 2$ (since for $f(t)/\sigma_t \lesssim -2$, the events $S(t_i,\ i = 1, \ldots, n)$ and $S(t_1)$ occur simultaneously with a probability close to one, and for $\dot{f}(t)/\sigma_t \gtrsim 2$, the integrals (18) and (19) are practically zero regardless of the events mentioned);

2) the angle of incidence θ_1 is close to 90° (since in this case the molecules would collide with the peaks of the roughnesses and integrals such as $\int_{-\infty}^{f(t_1)}$ can be replaced by $\int_{-\infty}^{\infty}$. Actually, this means that for such incidence of the molecules the stochastic function $\xi(t)$ can be considered as a one-dimensional Poisson process which agrees with the theory of high-order excursions [6]).

Thus there is a very limited region $|\dot{f}(t)/\sigma_t| \lesssim 2$ where the approximation (19), (20) leads to error. If the roughness is slight, this region is small and has no practical effect on the calculation of integral characteristics. Rough calculations have shown that in the case of severe roughness ($\sigma_t \leq 1$) an error of

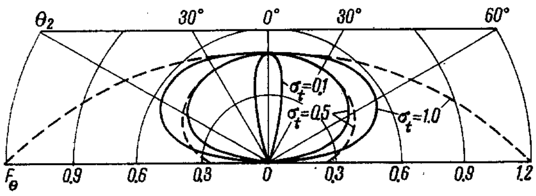

Fig. 5

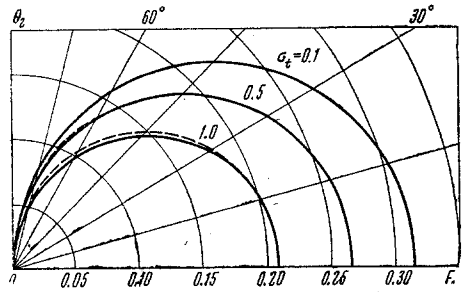

Fig. 6

10% or less is introduced into such interaction characteristics as the probability of single reflection and the accommodation coefficients for momentum and energy. In addition, the error mentioned tends to zero when $\theta_1 \to 90°$, and the approximation (19), (20) becomes applicable for any roughness.

Figures 2-6 give computed results obtained from Eq. (20) for cases where the reflection law F_0 is specular (Figs. 2-5) and diffuse (Fig. 6).

The first two figures show the dependence of the quantity F_1 on the vertical angle of incidence θ_1 for an isotropic surface with variances $\sigma_t^2 = 0.01$ (Fig. 2) and $\sigma_t^2 = 1$ (Fig. 3). As is clear, the scattering curve bears less resemblance to specular reflection as the variance increases and begins to develop "spikes" in the direction of the incident flux. In that case, the maximum spike is observed for those particles which are incident on the surface perpendicularly to the central line of the slope of the roughness in the direction of incidence.

Figure 4 shows the effect of anisotropy on the transform F_1. It shows the reflection curves with respect to the azimuthal angles φ_2 for the case of vertical incidence of particles on a weakly anisotropic surface ($\sigma_x / \sigma_y = 1.2$). For better visualization, the quantity $F_1 = F_1(\theta_2, \varphi_2)$ is replaced by the expression

$$F_\varphi = F_1(\theta_2, \varphi_2) \Big/ \int_0^{2\pi} F_1(\theta_2, \varphi_2)\, d\varphi_2$$

It is clear that for the case of an isotropic surface ($\sigma_x / \sigma_y = 1$) such a normalized transform should be represented graphically by a perfect circle. As is clear from the figure, this circle begins to elongate along the direction of maximum variance when anisotropy appears, with the elongation becoming increasingly greater as the angle θ_2 increases. As the anisotropy increases, this elongation intensifies, and the quantity F_φ for any angles $\theta_2 \neq \pi/2$ approaches a half-sum of δ-functions: $0.5\,[\delta(\varphi_2) + \delta(\varphi_2 - \pi)]$.

Similar relationships are also observed when the reflection law F_0 is diffuse; however, the effect is considerably weaker.

Figures 5 and 6, respectively, show a comparison of single reflection curves for specular and diffuse reflection laws F_0 calculated from approximation (20) and from [1] (dashed line). For simplicity, the case of a molecule vertically incident on an isotropic surface was selected. The quantity F_1 was replaced by the normalized expression

$$F_\theta = F_1(\theta_2, \varphi_2) \,/\, F_1(0, \varphi_2)$$

As is clear, divergence between the approximations begins at precisely those values of σ_t for which the approximation in [1] becomes inapplicable.

Using Eq. (20), one can calculate the probability of single reflection, the accommodation coefficients for momentum and energy, and other aerodynamic parameters.

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