Archives of Mechanics • Archiwum Mechaniki Stosowanej • 26, 5, pp. 787–794, Warszawa 1974

Soft sphere lattice scattering at oblique incidence

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THE REFLECTION of gas particles from a lattice of spherical atoms is studied. An analytic solution of the two-dimensional problem is obtained for small parameter ν specifying the potential barrier deviation from a vertical. The asymptotic approach enables us to split the real collective interaction into a sequence of pairwise collisions. First and second collisions are considered. Exit velocity, scattering indicatrix, momentum and energy exchange coefficients are found depending on ν, mass ratio μ, lattice stiffness parameter α_* and incidence angle θ_1.

Rozważono zagadnienie odbicia cząsteczek gazu od sieci kulistych atomów. Otrzymano rozwiązanie analityczne zagadnienia dwuwymiarowego dla małych wartości parametru ν określającego odchylenie bariery potencjału od pionu. Podejście asymptotyczne pozwala na rozłożenie rzeczywistego oddziaływania wzajemnego na szereg par zderzeń. Rozpatrzono pierwsze i drugie zderzenia. Wyznaczono prędkość cząsteczek po odbiciu, wskaźnik rozproszenia oraz współczynniki wymiany energii i pędu w zależności od współczynnika ν, stosunku mas μ, parametru sztywności sieci α_* oraz kąta padania θ_1.

Обсуждена проблема отражения молекул газа от решетки сферических атомов. Получено аналитическое решение двумерной проблемы для малых значений параметра определяющего отклонение барьера потенциала от вертикали. Асимптотический подход позволяет на разложение реального взаимодействия в ряд парных столкновений. Рассмотрены первые и вторые столкновения. Определены скорость молекул после отражения, коэффициент рассеяния и коэффициенты обмена энергии и импульса в зависимости от коэффициента ν, отношения масс μ, параметра жесткости решетки α_* и угла падения θ_1.

IN PAPERS [1a, 2, 3] the problem of gas atom reflection from a soft-sphere lattice was solved for atom incidence along the surface normal. At oblique incidence, the complicated picture of shadows and multiple collisions hampers making a sufficiently simple analytic theory. The qualitative idea of the solution structures needed to work out correct models can be given by the two-dimentional problem, where the shadow and multiple reflection effects are of a visible form. For hard atoms, such a problem has been solved in [4].

In this paper, the analytic solution of the two-dimensional problem is obtained to within $O(\nu)$, ν being the small parameter specifying the potential barrier deviation from a vertical. Some estimates of real ν by experimental data are given. The expansion in mass ratio μ has not, by contrast with [2, 3], been used. Both first and second collisions are taken into account. The momentum and energy exchange coefficients are calculated at incidence angles $\theta_1 = 0(15)75°$ for $\nu = 0; 0.1$; $\mu = 0; 0.25; 0.5$ and two values of lattice stiffness parameter α_*. Also obtained are asymptotic formulas for small α_*.

1. Effective inclination of potential

The hard sphere model does not provide the proper angular distribution of scattered particles. Therefore in [1–3] a slightly inclined barrier of a finite range was taken as the repulsive instead of the vertical potential. Over the short working range $r \in [r_{\min}, a_*]$ the potential was assumed to be representable as

$$U(r) = U'(a_*)(r-a_*)+O(1)(r-a_*)^2, \tag{1.1}$$

the inclination was specified by the small parameter

$$\nu = E_1[(1+\mu)a_*|U'(a_*)|]^{-1}, \tag{1.2}$$

E_1 being the impact energy, μ — atom mass ratio. The asymptotic approach makes it possible to solve the soft-sphere lattice scattering problem in an analytic form. The solution up to terms $O(\nu^2)$ proves to depend on the potential through the parameter ν only.

Let us estimate real values of ν on the basis of the results in [5–7] for the two most generally used models of repulsive potential:

$$U(r) = Kr^{-s}, \tag{1.3}$$

$$U(r) = A\exp(-\lambda r). \tag{1.4}$$

Parameters s, K or λ, A have been found for finite intervals Δr only. The effective inclination of potential in the range where U reaches the E_1 level can be determined by drawing a straight line through the points at which $U = E_1$ and $U = E_1/2$ — i.e., by the equations

$$U(r_{\min}) = E_1, \quad U[(r_{\min}+a_*)/2] = E_1/2. \tag{1.5}$$

Then, $|U'(a_*)| = E_1/(a_*-r_{\min})$, so that

$$\nu_0 = \nu(1+\mu) = 1-r_{\min}/a_*. \tag{1.6}$$

The Eqs. (1.5) result in $r_{\min}$ and a_*. In the case of (1.3):

$$\nu_0 = (2^{1+\frac{1}{s}}-2)/(2^{1+\frac{1}{s}}-1), \tag{1.7}$$

in the case of (1.4):

$$\nu_0 = \left[1+\frac{\ln(A/E_1)}{2\ln 2}\right]^{-1}. \tag{1.8}$$

The values of ν_0 found by (1.7), (1.8) are given in Table 1.

Table 1.

s	5	6	7	8	9	10	11	12
ν_0	0.229	0.197	0.172	0.153	0.138	0.126	0.115	0.106
A/E_1	200	400	1000	2000	3000	4000	6000	8000
ν_0	0.207	0.188	0.167	0.154	0.148	0.143	0.138	0.134

Figure 1 shows the potential curve (1.4) with typical values of parameters $\lambda = 4\text{Å}^{-1}$, $A = 4400$ eV in the range with upper point $E_1 = 2$ eV; $r_{\min} = 1.924\text{Å}$, $a_* = 2.272\text{Å}$,

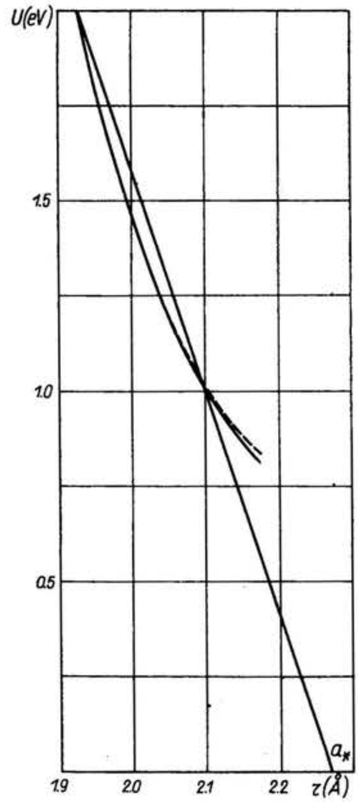

FIG. 1.

$\nu_0 = 0.153$. The dotted line is the curve (1.3) with $s = 8$ crossing the point (r_{min}, E_1); for this $K = 375.7$ eV. When $E_1/2 < U < E_1$, the plots coincide. The inclined barrier approximates these potentials sufficiently well within $0.4\,E_1 \lesssim U \leqslant E_1$. Below this interval, it is an extrapolation providing the finite range of potential.

Hence the parameter ν really proves to be sufficiently small to justify the asymptotic approach. Dealing with specific gases and surfaces, we can find ν and a_* by means of (1.5) using the Tables from [6, 7] for the parameters of potential (1.4) in the form

(1.9) $$U(r) = F_0 \varrho \exp[(R-r)/\varrho], \quad F_0 = \text{const},$$

and the combining rule

(1.10) $$2R_{ij} = R_{ii} + R_{jj}, \quad 2\varrho_{ij} = \varrho_{ii} + \varrho_{jj}.$$

2. Solution of two-dimensional problem

Let atom centres of the upper lattice layer be arranged along axis t at points $0, \pm 1, \pm 2, \ldots$ Drawing circles of radius a_* at these centres for $a_* \geqslant 0.5$, we have a continuous periodic surface on which gas atom centres occur at moments of encounter.

Let $\sin\alpha_* = 1/(2a_*)$, $0 \leqslant \alpha^* \leqslant \pi/2$. Encounter point $\bar{r}$, impinging velocity $\bar{u}_1$, and emerging velocity $\bar{u}$have the components

$$\bar{r} = \{a_* \sin\alpha, a_* \cos\alpha\}, \bar{u}_1 = \{-\sin\theta_1, -\cos\theta_1\}, \bar{u} = \{u\sin\theta, u\cos\theta\}.$$

The angles are counted from the normal $\bar{n}$, positive to the right, negative to the left, $-\alpha_* \leqslant \alpha \leqslant \alpha_*$, $0 \leqslant \theta_1 < \pi/2$, $-\pi/2 \leqslant \theta \leqslant \pi/2$.

In the coordinate system rotated through the angle θ_1, the problem of individual collision can be solved as at normal incidence. To within $0(\nu)$ we obtain:

$$\begin{aligned} u\sin\theta &= -\sin\theta_1 + \frac{2}{1+\mu}\cos(\alpha-\theta_1)\,[\sin\alpha + 2\nu\sin(\alpha-\theta_1)\cos(2\alpha-\theta_1)], \\ u\cos\theta &= -\cos\theta_1 + \frac{2}{1+\mu}\cos(\alpha-\theta_1)[\cos\alpha - 2\nu\sin(\alpha-\theta_1)\sin(2\alpha-\theta_1)]. \end{aligned} \tag{2.1}$$

The reflection structure connected with shadowing and multiple collisions depends on the interaction parameters. Taking into account double reflection, we can divide the plane (θ_1, α_*) into 5 specific parts (Fig. 2 in [4]): I — single reflection only, II — second

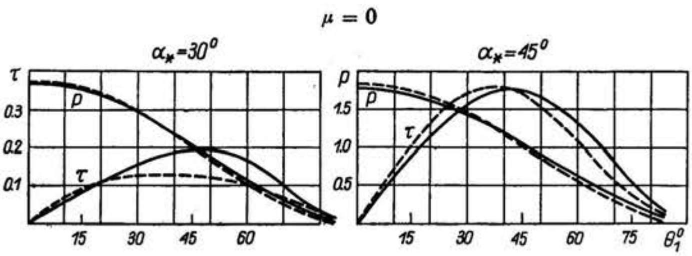

FIG. 2.

collisions with the left-hand atom, III — second collisions with the two neighbouring atoms, IV — shadowing and second collisions with the left-hand atom, V — shadowing and second collisions with the two neighbouring atoms. The single reflection range $\alpha_- < \alpha < \alpha_+$ in the general case is determined by

$$\alpha_- = \begin{cases} -\alpha_* \text{ in I}, \\ \alpha_1^- \text{ in II}-\text{V}, \end{cases} \qquad \alpha_+ = \begin{cases} \alpha_* \text{ in I, II}, \\ \alpha_1^+ \text{ in III, V}, \\ \alpha_s^+ \text{ in IV}, \end{cases} \tag{2.2}$$

where $\alpha_1^{\mp}$ are the first-collision boundaries, α_s^+ is the right-atom shadow boundary. These values have been studied in [4, 1b].

The scattering function is $V = V_1 + V_2$,

$$V_i = V_{i\theta}(\theta)\frac{1}{u_i(\theta)}\delta[u-u_i(\theta)], \quad i = 1, 2. \tag{2.3}$$

For the single scattering

$$V_{1\theta} = \frac{\cos(\alpha-\theta_1)}{2\sin\alpha_*\cos\theta_1|d\theta/d\alpha|}, \quad \theta_- \leqslant \theta \leqslant \theta_+, \tag{2.4}$$

and $u_1(\theta), \theta(\alpha)$ are determined by (2.1), together with $\theta_{\mp} = \theta(\alpha_{\mp})$ as soon as the single reflection boundaries (2.2) are known. Calculating the derivative $d\theta/d\alpha$ one obtains

$$V_{1\theta} = \frac{\cos(\alpha-\theta_1)}{4\sin\alpha_*\cos\theta_1} \cdot \frac{1-2\mu\cos2(\alpha-\theta_1)+\mu^2+2\mu\nu[1-\cos4(\alpha-\theta_1)]}{1+(2\nu-\mu)\cos2(\alpha-\theta_1)-2\mu\nu\cos4(\alpha-\theta_1)}. \tag{2.5}$$

For the double scattering $V_{2\theta}$ may be written as in (2.4), and $u_2(\theta), \theta(\alpha)$ have been found in [1b]. The range of θ is determined by the intervals $-\alpha_* \leqslant \alpha < \alpha_-$, $\alpha_+ < \alpha \leqslant \alpha_*$. Where the corresponding θ intervals overlap, the values of $V_{2\theta}$ are added.

Integrating V_i over $u_n > 0$ gives the probability of i fold scattering:

$$N_i = \int V_{i\theta}d\theta = \frac{a_*}{\cos\theta_1}\int\cos(\alpha-\theta_1)d\alpha,$$

(2.6)

$$N_1 = \frac{1}{2\sin\alpha_*\cos\theta_1}[\sin(\alpha_+-\theta_1)-\sin(\alpha_--\theta_1)], \quad N_2 = 1-N_1.$$

Table 2 contains N_1 for $\alpha_* = 30°, 45°$; $\mu = 0; 0.25; 0.5$; $\nu = 0, 0.1$; $\theta_1 = 0(15)75°$.

Table 2. N_1

α_*°	μ	ν	θ_1^0: 0	15	30	45	60	75
30	0	0	1	0.979	0.942	0.913	0.921	0.965
		0.1	0.744	0.857	0.839	0.835	0.873	0.943
	0.25	0	0.958	0.932	0.890	0.867	0.887	0.947
		0.1	0.706	0.803	0.769	0.764	0.815	0.913
	0.5	0	0.841	0.851	0.822	0.809	0.846	0.925
		0.1	0.601	0.609	0.682	0.679	0.746	0.875
45	0	0	0.846	0.853	0.875	0.911	0.947	0.976
		0.1	0.704	0.719	0.768	0.865	0.916	0.961
	0.25	0	0.756	0.770	0.813	0.876	0.922	0.963
		0.1	0.612	0.631	0.695	0.814	0.877	0.940
	0.5	0	0.636	0.659	0.728	0.833	0.892	0.947
		0.1	0.496	0.521	0.602	0.755	0.830	0.915

3. Exchange coefficients

Writing tangential momentum τ, normal momentum p, and energy q exchange coefficients [2] as

$$\tau = \tau_1+\tau_2, \quad p = p_1+p_2, \quad q = q_1+q_2; \tag{3.1}$$

$$\tau_i = \tau_i^-+\tau_i^+, \quad p_i = p_i^-+p_i^+, \quad q_i = q_i^--q_i^+, \quad i = 1, 2; \tag{3.2}$$

one has

$$\tau_i^- = N_i\sin\theta_1\cos\theta_1, \quad p_i^- = N_i\cos^2\theta_1, \quad q_i^- = N_i\cos\theta_1; \tag{3.3}$$

$$\tau_i^+ = \cos\theta_1\int\limits_{u_n>0} V_i u\sin\theta d\bar{u} = a_*\int\cos(\alpha-\theta_1)u_i(\theta)\sin\theta d\alpha,$$

(3.4) $$p_i^+ = \cos\theta_1 \int_{u_n>0} V_i u \cos\theta d\bar{u} = a_* \int \cos(\alpha-\theta_1) u_i(\theta)\cos\theta d\alpha,$$

$$q_i^+ = \cos\theta_1 \int_{u_n>0} V_i u^2 d\bar{u} = a_* \int \cos(\alpha-\theta_1) u_i^2(\theta) d\alpha.$$

For $i = 1$, the integrals (3.4) are taken by means of (2.1) in an analytic form. Combining the impinging and emerging fluxes, we obtain:

$$\tau_1 = 2a_*(1+\mu)^{-1}[(S_0-2\nu S_1)\sin\theta_1-(C_0-2\nu C_1)\cos\theta_1],$$

(3.5) $$p_1 = 2a_*(1+\mu)^{-1}[(C_0-2\nu C_1)\sin\theta_1+(S_0-2\nu S_1)\cos\theta_1],$$

$$q_1 = 4a_*\mu(1+\mu)^{-2}(S_0-2\nu S_1),$$

where

$$S_0 = [\sin(\alpha_+-\theta_1)-\sin(\alpha_--\theta_1)]-\frac{1}{3}[\sin^3(\alpha_+-\theta_1)-\sin^3(\alpha_--\theta_1)],$$

(3.6) $$C_0 = \frac{1}{3}[\cos^3(\alpha_+-\theta_1)-\cos^3(\alpha_--\theta_1)],$$

$$S_1 = \frac{2}{3}[\sin^3(\alpha_+-\theta_1)-\sin^3(\alpha_--\theta_1)]-\frac{2}{5}[\sin^5(\alpha_+-\theta_1)-\sin^5(\alpha_--\theta_1)],$$

$$C_1 = \frac{1}{3}[\cos^3(\alpha_+-\theta_1)-\cos^3(\alpha_--\theta_1)]-\frac{2}{5}[\cos^5(\alpha_+-\theta_1)-\cos^5(\alpha_--\theta_1)].$$

For $i = 2$ the integrals (3.4) are taken over the intervals $-\alpha_* \leqslant \alpha < \alpha_-$, $\alpha_+ < \alpha \leqslant \alpha_*$, using the corresponding functions $u_2(\theta)$, $\theta(\alpha)$ from [1b]. Then τ_2, p_2, q_2 are calculated by (3.2), (3.3).

Figs. 2–4 show the dependence of τ, p, q on θ_1 for

$$\alpha_* = 30°; 45°; \quad \mu = 0; 0.25; 0.5; \quad \nu = 0; 0.1\ (-, --).$$

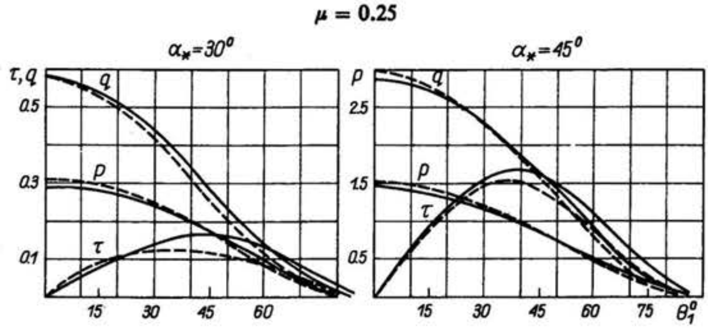

FIG. 3.

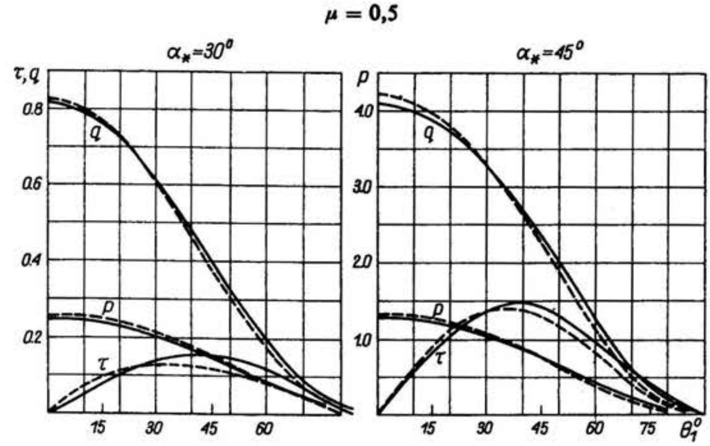

FIG. 4.

4. Asymptotics for small α_*

With decreasing α_*, the shadowing and multiple collisions effects are reduced. When α_* is sufficiently small, we are in the single reflection range I where, according to (2.2), $\alpha_- = -\alpha_*$, $\alpha_+ = \alpha_*$. There $N_1 = 1$ and (3.5), (3.6) result in:

$$\tau = \frac{\sin 2\theta_1}{(1+\mu)}\left\{\frac{2}{3}\sin^2\alpha_* - 2\nu\left[\left(\frac{5}{3}\sin^2\alpha_* - \frac{8}{5}\sin^4\alpha_*\right) + \cos^2\theta_1\left(1 - 4\sin^2\alpha_* + \frac{16}{5}\sin^4\alpha_*\right)\right]\right\},$$

$$p = \frac{1}{(1+\mu)}\left\{\left[\frac{2}{3}\sin^2\alpha_* + \frac{2}{3}\cos^2\theta_1(3 - 2\sin^2\alpha_*)\right] - 4\nu\left[\left(\frac{1}{3}\sin^2\alpha_* - \frac{2}{5}\sin^4\alpha_*\right) + \cos^2\theta_1\left(1 - \frac{11}{3}\sin^2\alpha_* + \frac{16}{5}\sin^4\alpha_+\right) - \cos^4\theta_1\left(1 - 4\sin^2\alpha_* + \frac{16}{5}\sin^4\alpha_*\right)\right]\right\},$$

(4.1)

$$q = \frac{4\mu}{(1+\mu)^2}\cos\theta_1\left\{\left[\sin^2\alpha_* + \cos^2\theta_1\left(1 - \frac{4}{3}\sin^2\alpha_*\right)\right] - 4\nu\left[(\sin^2\alpha_* - \sin^4\alpha_*) + \cos^2\theta_1\left(1 - \frac{14}{3}\sin^2\alpha_* + 4\sin^4\alpha_*\right) - \cos^4\theta_1\left(1 - 4\sin^2\alpha_* + \frac{16}{5}\sin^4\alpha_*\right)\right]\right\}.$$

The boundary of range I for $\alpha_{*1}^- \to 0$ ($\theta_1 \to \pi/2$) has the simple asymptotic form:

(4.2)
$$\alpha_{*1}^- = \frac{1-\mu}{3+\mu}\left(\frac{\pi}{2} - \theta_1\right).$$

Since α is included within a small interval near zero, we have from (2.1):

$$\mathrm{tg}\theta = -\frac{1+\mu}{1-\mu}\mathrm{tg}\theta_1\left[1-2(\alpha-\nu\sin 2\theta_1)\left(\frac{\mathrm{tg}\theta_1}{1-\mu}+\frac{\mathrm{ctg}\theta_1}{1+\mu}\right)+O(\alpha^2)\right]. \tag{4.3}$$

The emerging velocity and the scattering indicatrix are insignificantly simplified. The asymptotic expressions of the exchange coefficients in I are simply obtained from (4.1)

$$\begin{aligned} \tau &= \frac{2\sin 2\theta_1}{3(1+\mu)}(\alpha_* - 3\nu\cos^2\theta_1),\\ p &= \frac{2}{(1+\mu)}\left[\cos^2\theta_1+\frac{\alpha_*^2}{3}(1-2\cos^2\theta_1)-\frac{\nu}{2}\sin^2 2\theta_1\right],\\ q &= \frac{4\mu\cos\theta_1}{(1+\mu)^2}\left[\cos^2\theta_1+\frac{\alpha_*^2}{3}(3-4\cos^2\theta_1)-\nu\sin^2 2\theta_1\right]. \end{aligned} \tag{4.4}$$

Note that decreasing α_* for a fixed ν enlarges the collective interaction zone and the arguments (see [1a]) leading to the identity V_* with V_1 become invalid. Therefore the parameter ν in (4.4) must decrease together with α_*, and also sufficiently rapidly. Decreasing α_* before ν requires a further analysis of the collective interaction zone.

Asymptotics by α_* makes it possible to obtain also an analytic solution of the three-dimensional problem.

References

1. R. G. BARANTSEV, N. I. MERKULOVA, *Soft sphere lattice scattering*. a) I. *First approximation at normal incidence*, Vestnik of the Leningrad University, 7, 82–88, 1972. b) III. *Oblique incidence. Two-dimensiona problem* [in Russian], Ibid., 7, 90–95, 1974.
2. R. G. BARANTSEV, *Some problems of gas-solid surface interaction*. Progress in Aerospace Science, **13**, 1–80, 1972.
3. R. G. BARANTSEV, *Soft sphere lattice scattering*, Proc. 8th Symp. Rarefied Gas Dynamics, 1974.
4. R. G. BARANTSEV, V. G. LANDMAN, *Two-dimensional problem of atom reflection from hard disk lattice* [in Russian], Rarefied Gas Aerodynamics, Leningrad University, **7**, 60–70, 1974.
5. V. B. LEONAS, *Studies of short-range intermolecular forces* [in Russian], Progress in Phys. Sci., **107**, 1, 29–56, 1972.
6. Ch. BUTTERFIELD, E. H. CARLSON, *Ionic soft sphere parameters from Hartree-Fock-Slater calculations*, J. Chem. Phys., **56**, 10, 4907–4911, 1972.
7. K. G. SPEARS, *Repulsive potentials of atomic ions, atoms, and molecules*, J. Chem. Phys., **57**, 5, 1842–1849, 1972.

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Received September 5, 1973.