



# New modeling of scattering behaviors of argon atoms on tungsten substrate

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## ARTICLE INFO

### Article history:

Received 6 May 2011

Received in revised form 2 August 2011

Accepted 7 August 2011

Available online 19 August 2011

### Keywords:

Molecular dynamics

Maxwell distribution

Argon–tungsten interactions

Morse potential

Statistical analysis

## ABSTRACT

In this study argon beam–tungsten surface scattering processes were investigated numerically by applying molecular dynamics simulations. Energy transfer, momentum change and the scattering processes of argon gas atoms from the W(110) surface were discussed. The molecular dynamics results showed that Maxwell boundary conditions fail to describe the behaviors of a high mean kinetic energy argon beam impinging on a tungsten surface. A new three-dimensional model of argon–tungsten interaction was thus proposed, and its results proved to be in line with experimental and theoretical results that have been obtained previously by other researchers.

Specifically, we developed a method for the normalization of the parameters of a gas beam scattered by a metal surface. We found that the ratio of the average velocity of the scattered beam to the appropriate root mean square deviation (RMSD) allowed us to determine whether the distribution of the scattered atoms was Maxwellian or not. We found that the shape of the functions representing the angular distributions of the scattered Ar atoms could be determined using the ratio of the RMSD of an angle (azimuthal or polar) of the scattered beam to the RMSD of a uniform distribution. The distribution of the azimuthal angle of the scattered atoms was found to be uniform regardless of the incident's kinetic energy, when the incident of the beam on the surface was normal.

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## 1. Introduction

Currently, the study of thermal transport processes in nanoscale systems is a priority within the field of modern science. The importance of these investigations is due to the downscaling of electronic devices, as well as their cooling systems. During studies of fluid behavior around or inside a microsystem (such as micro-cavity or micro-motor systems) researchers are interested in processes within the fluid or near the fluid–solid boundary rather than processes inside the solid microsystem. There is therefore no reason to create an accurate molecular model of the solid microdevice itself, which would normally involve a much greater number of atoms than for the fluid surrounding it.

Particle codes such as particle-in-cell [1] and direct simulation Monte Carlo [2] have been used with success for the simulation of rarefied gas flows. This is due to their ability to handle complex flow geometries and kinetic systems involving inelastic collisions and chemical reactions. As such, much effort has been devoted to developing a realistic model of intermolecular collision processes. However, an important issue in modeling a realistic flow involves determining the accurate scattering model of the gas and surface interaction.

The energy transfer and the scattering of rarefied gases from different surfaces have been the subject of a series of studies. For example, Maxwell [3], in his study of gas–surface interactions, proposed a simple model where a gas impinging on a surface is scattered into two fractions, one that reflects specularly and exchanges no energy and another that accommodates completely and desorbs with an equilibrium distribution. Other studies of gas–surface interactions have focused on determining the thermal accommodation coefficients [4] by applying experimental techniques that permit a greater control over the different conditions: Weinberg and Merrill [5] determined angular distributions for gas atoms scattered by a single-crystal W(110) surface; and Janda et al. [6] measured velocity distributions for argon atoms scattering from a clean, polycrystalline tungsten surface. The experimental results of the second study allowed the researchers to relate the average kinetic energy of scattered argon atoms to the average incident kinetic energy, as well as to the surface temperatures. In other recent representative studies, Fan and Manson [7] proposed theoretical explanations for argon atoms scattering from a self-assembled monolayer on Ag(111). Furthermore, Gibson et al. [12] conducted a detailed study of Ar scattering from an ordered 1-decanethiol–Au(111) monolayer.

While there are many publications related to gas–surface interactions, their results must first be adapted before they can be used as boundary conditions to describe the gas flow in micro- and nanosystems. Detailed experimental studies of fluid flow and

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gas–surface collisions in such systems are very time and resource consuming. However, recent achievements in computer simulation methods have made it possible to investigate effects on the molecular level, thereby achieving a reduction in the expenses of the development process. One of the numerical methods that facilitate the study of molecular interactions is molecular dynamics (MD). This method is based on fundamental principles of classical mechanics where the force fields between all atoms involved in a simulated system are described, thus creating precise models of micro- and nano-scale systems. Consequently, the implementation of the method requires powerful computers.

In this paper, the MD method was applied to study the argon gas scattering processes on a W(1 1 0) surface. The MD approach made it possible to precisely describe the interaction between argon gas and tungsten.

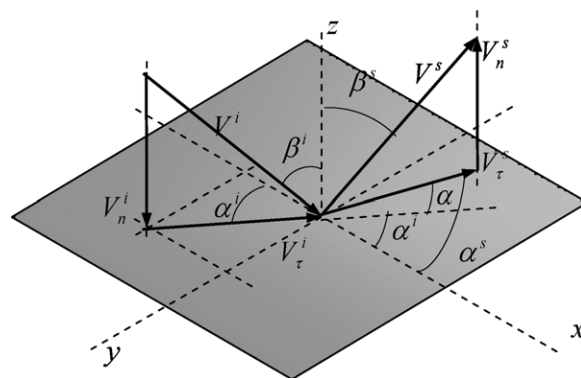
The aim of this work was to develop an algorithm allowing one to describe the obvious relations between the parameters of the incident and the scattered gas beams. The method applied in the present paper can be simply expressed as the bombing of a tungsten surface with argon atoms, where further analysis of the scattered atoms' trajectories was conducted. Analysis of both angular distributions and distributions of velocities of scattered atoms were performed using mean values and root mean square deviations (RMSDs). This combination provided complete information regarding the scattering process. For example, if the RMSD of the azimuthal angle of the scattered atoms was small (large) then we could conclude that the scattering was more specular (diffusive). In order to determine the relative size of the RMSD, we normalized the RMSDs by the corresponding mean value ( $\sigma_V/\mu_V$ ) in the case of velocity distributions, and the RMSD corresponding to the uniform distribution ( $\sigma_{\text{ang}}/\sigma_{\text{uni}}$ ) in the case of angular distributions. We observed that the relation  $\sigma_V/\mu_V$  tended towards 0.42 with a decreasing of the incident beam energy. Furthermore, when  $\sigma_V/\mu_V$  approached the limiting value, the distribution of velocities of the scattered Argon atoms became Maxwell, while the angular distribution became uniform when  $\sigma_{\text{ang}}/\sigma_{\text{uni}}$  reached its limiting value of 1, and Gaussian otherwise.

## 2. Methodology and computation

The physical system investigated in this study consisted of tungsten W(1 1 0) substrate with a temperature of  $T_{\text{surf}}$  and argon atoms with an initial velocity vector magnitude  $V^i$  and velocity vector direction determined by the azimuthal and polar angles  $\alpha^i$  and  $\beta^i$ , respectively. The simulation procedure consisted of a substrate bombardment of argon atoms, after which the scattered atoms' parameters  $V^s$ ,  $\alpha^s$  and  $\beta^s$  were determined (Fig. 1).

The theoretical research was performed numerically by using the MD simulation method. MD is a form of computer simulation in which atoms are allowed to interact for a period of time by approximations of known physics, giving a view of the motion of the atoms. All simulations described in this study were performed using a Fortran program developed by the authors.

In order to evaluate the gas scattering effects, we took as our prototypical system incidents of collimated, monoenergetic beams of argon atoms on the (1 1 0) face of a tungsten crystal. The intensity of an incident beam was  $2 \times 10^5$  Pa. The surface substrate consisted of three layers of tungsten atoms, where the sizes in the X, Y and Z directions were  $85.5\text{\AA} \times 58.6\text{\AA} \times 7\text{\AA}$ , respectively. The atoms that comprised the lower layer were held fixed in their equilibrium lattice positions, while the atoms in other two layers were permitted to move according to the appropriate classical equations of motion.



**Fig. 1.** Coordinate system, where  $\alpha^i$  and  $\beta^i$  – incident azimuthal and polar angles, respectively;  $\alpha^s$  and  $\beta^s$  are scattered beam's azimuthal and polar angles, respectively;  $\alpha = \alpha^s - \alpha^i$  – azimuthal angle change caused by the scattering of the beam;  $V_n^i$  and  $V_\tau^i$  – normal and tangential velocity components of the incident beam;  $V_n^s$  and  $V_\tau^s$  – normal and tangential velocity components of the scattered beam.

The interactions among tungsten atoms were taken as being sums of pairwise Morse potential:

$$\Phi_{W-W} = \begin{cases} D_W [e^{-2B_W(r-R_W)} - 2e^{-B_W(r-R_W)}], & 0 < r < 2.3R_W \\ 0, & r \geq 2.3R_W \end{cases}, \quad (1)$$

where the potential's parameters were [8]:  $D_W = 0.9906$  eV,  $B_W = 14.116$  nm<sup>-1</sup>,  $R_W = 0.3032$  nm.

To describe the interaction between an argon and tungsten atom, we applied the Lennard-Jones potential function:

$$\Phi_{W-Ar} = \begin{cases} 4\varepsilon_{WAr} \left[ \left( \frac{R_{WAr}}{r} \right)^{12} - \left( \frac{R_{WAr}}{r} \right)^6 \right], & 0 < r < 2.5R_{WAr} \\ 0, & r \geq 2.5R_{WAr} \end{cases}, \quad (2)$$

where the parameter values used were:  $\varepsilon_{WAr}/k_B = 25.17$  K,  $R_{WAr} = 2.93$  Å.

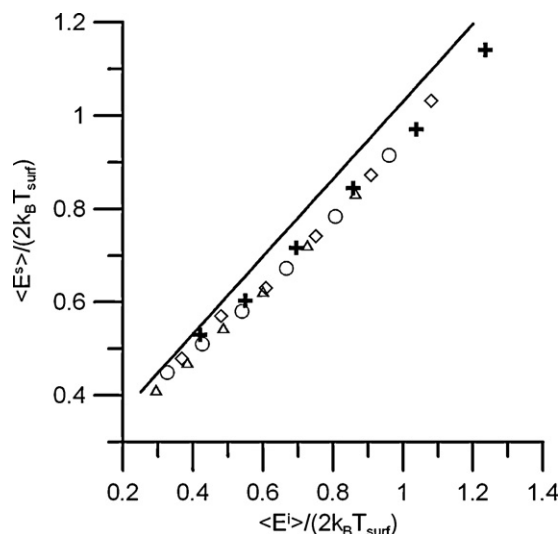
The Lennard-Jones 6–12 potential was also used to describe argon–argon interactions, with the parameter  $\varepsilon_{Ar}/k_B = 119.18$  K.

The initial conditions for trajectories involving this surface were selected so as to reflect the thermal fluctuations appropriate to the given system temperature. We generated the set of atomic positions at time equal to zero on the basis of a thermally biased random walk of those atoms in the system for which motion was allowed.

The initial lateral position for the impinging atom was selected at random on a plane 17 Å above the average position of the uppermost solid layer. In order to model the scattering of a velocity-selected, collimated beam, the initial momentum of the incident atom was taken to be the same for each trajectory of a given set. An integration of equations of motion was performed using the second order velocity Verlet scheme [8]. The time step for the current computations was  $\Delta t = 10^{-16}$  s – smaller than the characteristic time of atom interactions. The computational process was continued until all the argon atoms were retired no more than 17 Å from the surface atoms (i.e. until all the gas atoms were within the force field of the tungsten atoms). Gas atoms that went beyond this distance were excluded from the system, and information on their velocities and coordinates were stored in a file. By excluding these scattered atoms, the time required for the calculation was reduced, and the randomization of velocities of argon atoms as a consequence of their collision with each other was prevented.

## 3. Results and discussion

The current investigations were conducted for various angles of incidents (from  $\beta^i = 0^\circ$  to  $70^\circ$  with  $5^\circ$  steps), a series of surface



**Fig. 2.** Mean energy of scattered atoms versus energy of impinging atoms at  $\beta^i = 45^\circ$ . +,  $T_{\text{surf}} = 350$  K;  $\diamond$ ,  $T_{\text{surf}} = 450$  K;  $\circ$ ,  $T_{\text{surf}} = 400$  K;  $\Delta$ ,  $T_{\text{surf}} = 500$  K; solid line – results from [6].

temperatures ( $T_{\text{surf}} = 350$  K, 400 K, 450 K, 500 K), and varied velocities of impinging Ar atoms (from  $V^i = 100$  m/s to 1600 m/s with 50 m/s steps). A total of 1920 cases were computed.

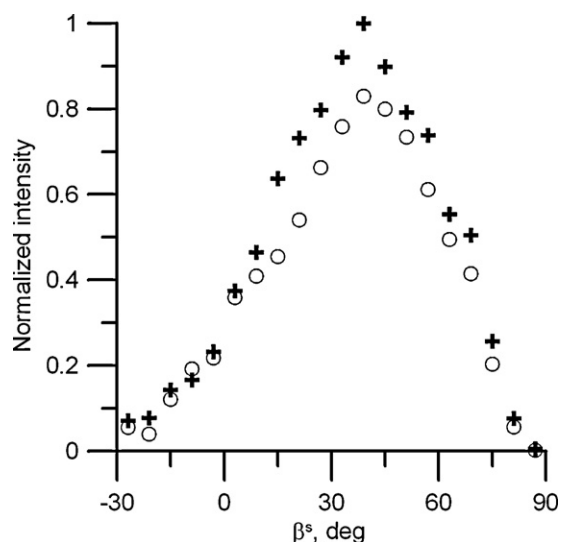
Every analytical or numerical study based on mathematical models has assumptions. Consequently, results of such works must be proven by comparing experimental results. Fig. 2 shows the correlation of the mean kinetic energies of the impinging atoms with the mean kinetic energy of the beam scattered by the tungsten surface. A solid line corresponds to the linear relation between parameters, mentioned above, following Janda et al. [6]. Data represented by various symbols show results obtained in the current study corresponding to the set of incident energies and surface temperatures, where the angle of the incidents was  $\beta^i = 45^\circ$ ; these data points were approximated by the following function:

$$\langle E^s \rangle = b_B \langle E^i \rangle + b_S(2k_B T_{\text{surf}}), \quad (3)$$

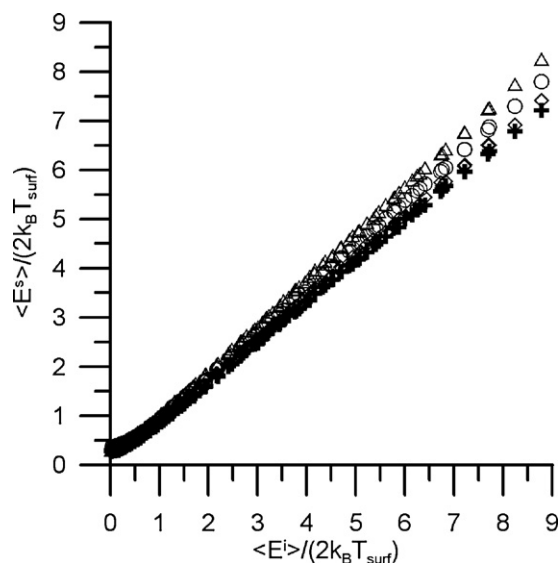
where  $k_B$  was the Boltzmann's constant, and  $b_S = 0.77$  and  $b_B = 0.18$  were the proportionality factors. Analysis of Eq. (3) allowed us to conclude that if the energy of the incident beam was less than  $b_S(2k_B T_{\text{surf}})/(1 - b_B)$ , then the surface transferred energy to the gas ( $E^S > E^i$ ), otherwise the gas gave up energy to the surface ( $E^i > E^S$ ).

The difference between the experimental data and the calculated results did not exceed 9%; this difference can be explained by the fact that even the best MD models are a rough approximation of real processes. Also, it should be noted that we used monocrystalline tungsten, while Janda et al. [6] used polycrystalline tungsten, and that the simulated substrate was ideal, i.e. it had no irregularities or scratches, while real substrate may have some faults. Based on the above, we conclude that achieving a 9% difference is a strong result.

Another important parameter of the gas–surface interaction was the momentum change of the atoms, which was characterized by an angular distribution of scattered atoms. Fig. 3 presents the distributions of the polar angle of the scattered atoms. Circles and crosses correspond to two cases of surface temperature,  $T_{\text{surf}} = 350$  K and  $T_{\text{surf}} = 500$  K, respectively. Furthermore, the temperature and incident angle of the argon beam were equal to  $T_G = 295$  K and  $\beta^i = 45^\circ$ , respectively. As can be seen, the argon scattering distribution peaks increased in intensity with the increase in surface temperature. This finding is in line with the results of Weinberg and Merrill [5].



**Fig. 3.** Ar scattering from W(110) at  $T_G = 295$  K and incident angle  $\beta^i = 45^\circ$ . +,  $T_{\text{surf}} = 500$  K;  $\circ$ ,  $T_{\text{surf}} = 350$  K.

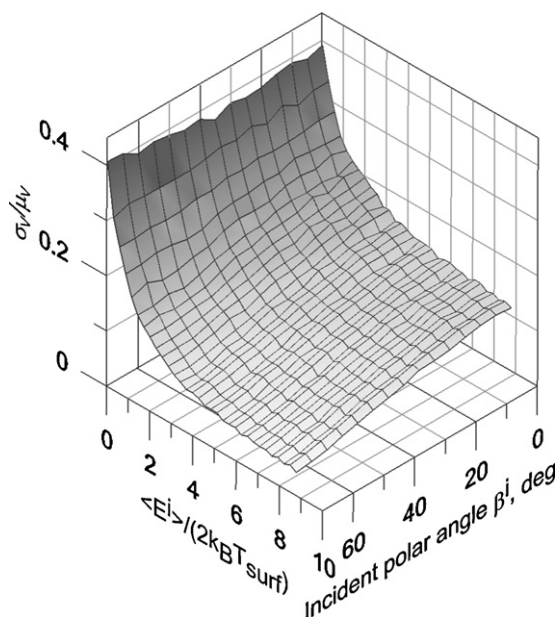


**Fig. 4.** Mean energy of scattered atoms versus energy of impinging Ar atoms. +,  $\beta^i = 0^\circ$ ;  $\diamond$ ,  $\beta^i = 20^\circ$ ;  $\circ$ ,  $\beta^i = 40^\circ$ ;  $\Delta$ ,  $\beta^i = 60^\circ$ .

Fig. 4 shows the average energy of the scattered beam as a function of incident beam energy  $\langle E^i \rangle$  for different values of the incident angle  $\beta^i$  of the beam. It is clear that all plots presented in Fig. 4 have two regions: (1) a linear region, where the mean energy of the scattered atoms linearly depended on the incident energy and (2) a nonlinear region, corresponding to relatively low energies of impinging Ar atoms, where the mean energy of the scattered atoms were independent of the incidents' energy. It should be noted that the slope of the linear regions on the plots shown in Fig. 4 increases with increasing incident angles of Ar atom beams. The same effect was also noted by Agrawal and Raff [9].

If the distribution of random numbers corresponded to a Maxwell distribution, the relationship between RMSD  $\sigma$  and the mean value  $\mu$  would be described by the following relation (see e.g. [10]):

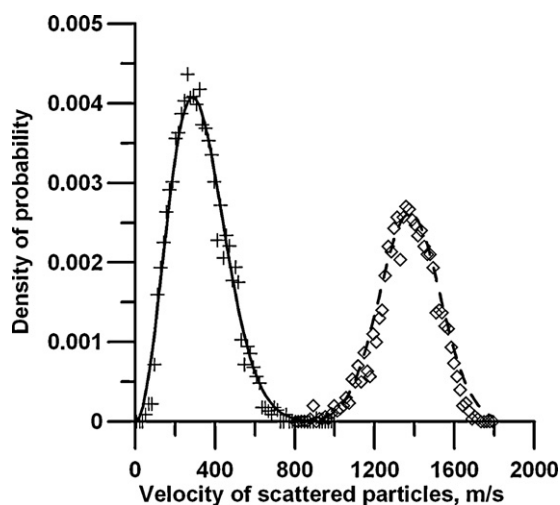
$$\frac{\sigma}{\mu} = \frac{1}{2} \sqrt{\frac{3\pi - 8}{2}} \approx 0.42 \quad (4)$$



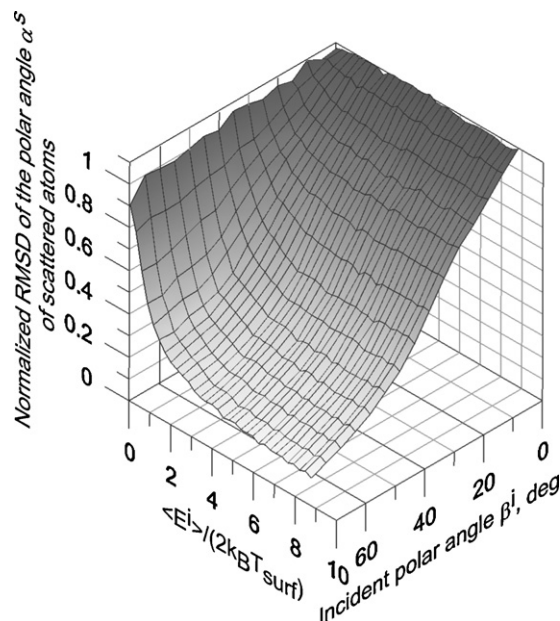
**Fig. 5.** Root mean square deviation of scattered atom's velocities  $\sigma_V$  over mean velocity of scattered atoms  $\mu_V$  versus kinetic energy impinging atoms.

The ratio  $(\sigma_V/\mu_V)$  of RMSD to the mean velocity of the atoms scattered by the surface as a function of incident beam energy is presented in Fig. 5. It can be seen that the distribution of velocities of scattered argon atoms tended towards a Maxwell distribution, as  $\sigma_V/\mu_V$  approached 0.42 (shown in Eq. (4)), with decreasing incident energy regardless of the incident polar angle  $\beta^i$ . Fig. 6 shows that the velocities of scattered argon atoms having low (high) incident energy were distributed according to a Maxwell distribution (shown by a solid (dashed) line and crosses (diamonds)). Taking into account the ratio  $E_{min}^i \leq \varepsilon_{WAr} \approx 0.095$  (where  $E_{min}^i$  was the minimal value of the kinetic energy of the impinging beam considered in this paper), one can conclude that Ar atoms with kinetic energy  $E^i \leq \varepsilon_{WAr}$  sank into the potential well, induced by the surface atoms, and were thus scattered by the surface, regardless of the initial conditions. A similar effect was mentioned by Fan and Manson [7].

Both polar and azimuthal angles of the scattered atoms were varied within ranges of  $[-\pi/2; \pi/2]$ , thus the normalized RMSD



**Fig. 6.** Density of probability of  $V^s$ .  $T_{surf} = 350$  K,  $\beta^i = 20^\circ$ ,  $V^i = 100$  m/s;  $\diamond$ ,  $\beta^i = 20^\circ$ ,  $V^i = 1500$  m/s; solid line – Maxwell distribution; dashed line – normal distribution.

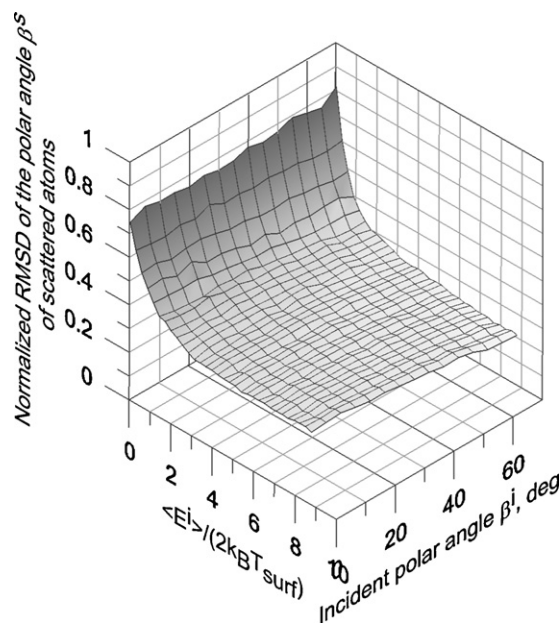


**Fig. 7.** Normalized root mean square deviation  $\sigma_\alpha$  of the azimuthal angle  $\alpha^s$  of scattered atoms versus kinetic energy of impinging atoms and incident polar angle.

corresponding to a uniform distribution for random numbers within this range was [11]:

$$\sigma_{uni} = \frac{b-a}{\sqrt{12}} = \frac{180}{\sqrt{12}} = 30\sqrt{3} \quad (5)$$

RMSDs of the scattering angles  $\alpha^s$  and  $\beta^s$  as presented in Figs. 7 and 8, respectively, were normalized by the  $\sigma_{uni}$  from Eq. (5). Based on the results shown in Fig. 7, we concluded that the mean azimuthal angle of the scattered beam  $\alpha^s$  was independent of incident kinetic energy and incident angle  $\beta^i$  when an atom's beam impinged normally on the surface. Fig. 8 presents correlations similar to those shown in Fig. 7, but for the polar angle  $\beta^s$  of the scattered beam.



**Fig. 8.** Normalized root mean square deviation  $\sigma_\beta$  of the polar angle  $\beta^s$  of scattered atoms versus kinetic energy of impinging atoms and incident polar angle.



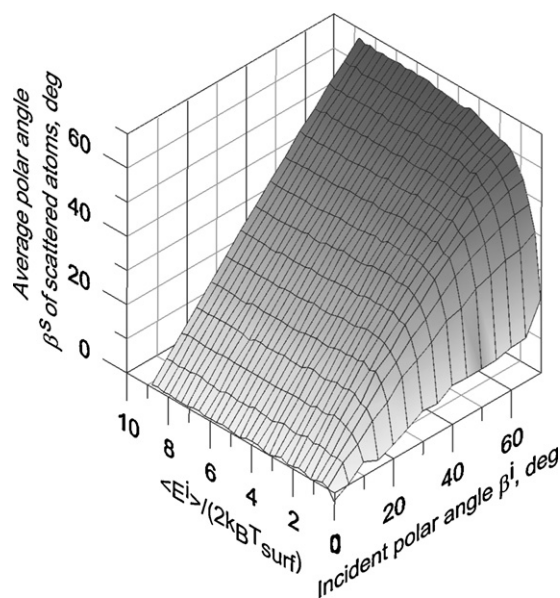


Fig. 9. Average polar angle  $\beta^s$  of scattered atoms versus kinetic energy of impinging atoms and incident polar angle.

Fig. 9 illustrates the correlation of the average polar angle  $\beta^s$  of the scattered atoms with incident kinetic energy and polar angle  $\beta^i$ . The results show that an increase in incident energy caused linearization of dependence between the incident and the scattered polar angle, while the average polar angle of the scattered argon atoms that had low incident energy tended towards zero.

It is clear that the distribution of the angle  $\beta^s$  did not become fully uniform (the angle did not become independent of other parameters) in the range of studied incident parameters of the Ar beam. On the other hand, the distribution of the angle  $\alpha^s$  became uniform (as shown by the cross symbols in Fig. 10a) when the incident beam had low energy ( $\langle E^i \rangle / (2k_B T_{\text{surf}}) \approx 0$ ) or was a normal falling beam ( $\beta^i \approx 0$ ), and became normal when the incidents had high energy (shown as crosses and a dashed line in Fig. 10b). The same effect is illustrated in Fig. 7. Comparing angle  $\beta^s$  in Figs. 10a and b, one can see that the scattering of Ar atoms was more elastic in the case of the high energy falling beam (Fig. 10b) than in the case of the low energy one (Fig. 10a). This issue can also be explained in terms of relation between  $E_{\text{min}}^i$  and  $\varepsilon_{\text{WAr}}$ .

Some results discussed above are contradictory to the Maxwell model of boundary conditions, as distributions of scattered particles can be described by the normal distribution function in the case of high incident energy. This is in contrast to the Maxwell model in which velocities satisfy the Maxwell–Boltzmann distribution.

By summarizing the results and discussion above, a new algorithm for better describing the scattering behaviors of argon atoms on tungsten substrate was proposed:

1. Parameters  $\beta^i$ ,  $\alpha^i$ ,  $V^i$  were determined from particle velocity components that reached stated boundary;
2. Parameters  $\mu_\beta$ ,  $\mu_V$ ,  $\sigma_\beta$ ,  $\sigma_V$  and  $\sigma_\alpha$  were determined by using charts that numerically represented the following functions  $\beta^s = f(V^i, \beta^i)$ ,  $V^s = f(V^i, \beta^i)$ ,  $\sigma_\beta = f(V^i, \beta^i)$ ,  $\sigma_V = f(V^i, \beta^i)$  and  $\sigma_\alpha = f(V^i, \beta^i)$ ;
3. If  $\sigma_\alpha \geq 0.9$  then angle  $\alpha$  was determined by using a random function with uniform distribution, otherwise  $\alpha$  was determined by using a sampling method based on the normal probability function with the RMSD value obtained in step 2 and mean value equal to 0.  $\alpha^s$  of the scattered particles was then defined as  $\alpha^s = \alpha + \alpha^i$ .

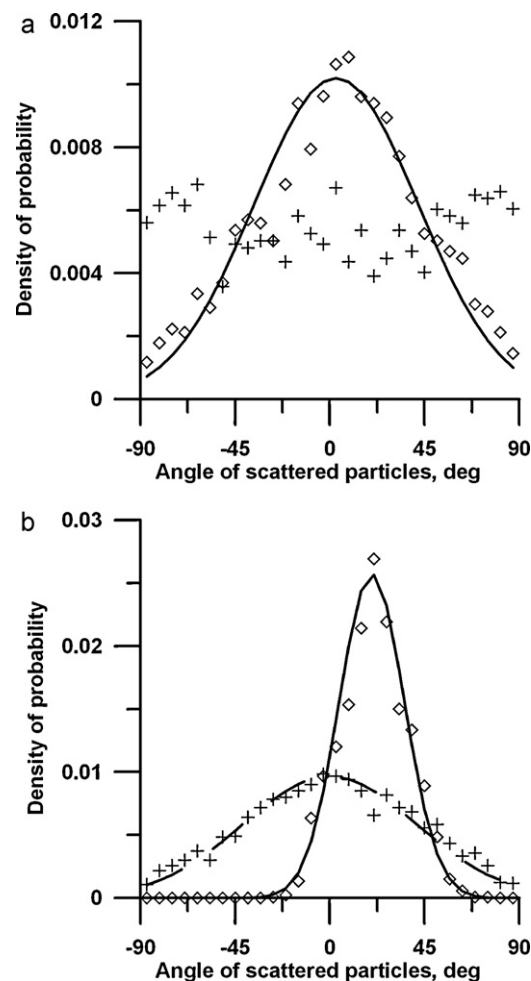


Fig. 10. (a) Density of probability of  $\beta^s$  and  $\alpha^s$ ,  $T_{\text{surf}} = 350$  K,  $\beta^i = 20^\circ$ ,  $V^i = 100$  m/s. +, distribution of  $\alpha^s$ ;  $\diamond$ , distribution of  $\beta^s$ ; solid line – normal distribution of  $\beta^s$ . (b) Density of probability of  $\beta^s$  and  $\alpha^s$ ,  $T_{\text{surf}} = 350$  K,  $\beta^i = 20^\circ$ ,  $V^i = 1500$  m/s. +, distribution of  $\alpha^s$ ;  $\diamond$ , distribution of  $\beta^s$ ; solid line – normal distribution of  $\beta^s$ ; dashed line – normal distribution of  $\alpha^s$ .

4. Parameter  $\beta^s$  was defined by using a sampling method based on the normal probability function with the RMSD  $\sigma_\beta$  value obtained in step 2 and mean values equal to the  $\mu_\beta$  of  $\beta^s$ .
5. The velocity of the scattered atom  $V^s$  was defined by using a sampling method based on a Maxwell distribution and mean value  $\mu_V$  when the incident atom's energy was  $E_{\text{min}}^i / \varepsilon_{\text{WAr}} \leq 1$ , and by using the normal probability function with the RMSD  $\sigma_V$  value obtained in step 2 and mean value  $\mu_V$  otherwise.

The presented algorithm was tested by replacing the tungsten substrate with a flat surface having a temperature of  $T_{\text{surf}} = 350$  K and applying the particle scattering law described by the above-mentioned algorithm. Incident velocity  $V^i$  and angle  $\beta^i$  of the tested case were  $V^i = 100 \dots 1600$  m/s and  $\beta^i = 20^\circ$ . We found that the proposed model was capable of reproducing the processes of the interaction between argon atoms and the tungsten substrate described above.

#### 4. Conclusion

In this work we developed a method for the normalization of the parameters of a gas beam scattered by a metal surface. We found that the ratio of the average velocity of the scattered beam to the appropriate RMSD allowed us to determine whether or not the distribution of the scattered atoms was Maxwell.

Furthermore, the applicability of the Maxwell boundary conditions was determined by using the incident energy. When the average incident kinetic energy of the Ar atoms in the beam approached zero ( $\langle E^i \rangle / (\varepsilon_{\text{WAr}}) \rightarrow 0$ ), the velocity distribution of the gas atoms in the scattered beam tended to a Maxwell distribution, while when  $\langle E^i \rangle / (\varepsilon_{\text{WAr}}) \gg 1$ , inapplicability of the Maxwell boundary conditions was observed. Furthermore, the angular distribution of the scattered gas atoms tended to be a uniform distribution with a decreasing kinetic energy of the impinging atoms. We found that the shape of the functions the represented angular distributions of the scattered Ar atoms could be determined using the ratio of the RMSD of an angle (azimuthal or polar) of the scattered beam to the RMSD of a uniform distribution ( $\sigma_{\text{ang}}/\sigma_{\text{uni}}$ ). The distribution of the azimuthal angle of the scattered atoms was uniform ( $\sigma_{\text{ang}}/\sigma_{\text{uni}} \approx 1$ ) regardless of the incident kinetic energy when incidents of the beam on the surface were normal.

Another important finding was that Eq. (3) cannot be used for the region corresponding to low kinetic energy of the impinging atoms due to the relation between potential energy induced by the tungsten atoms, and the kinetic energy of the impinging beam.

Lastly, we proposed an algorithm to describe how the data discussed above could be used as boundary conditions. Generally, this algorithm explains how to convert the experimental/simulation results into boundary conditions. Application of the newly proposed boundary conditions for Ar–W interactions provided a significant increase in calculation speed, which was implemented

by substituting atoms of a solid structure with surfaces following the gas scattering law described by the new proposed algorithm.

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