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New statistical boundary conditions for argon–tungsten interactions

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ABSTRACT

In this study, scattering processes of argon beam impinging on tungsten surface are investigated numerically by applying molecular dynamics (MD) simulations. Energy transfer, momentum change, and scattering processes of argon gas atoms from W(1 1 0) surface are discussed. A new model of argon–tungsten (Ar–W) interaction is proposed. Based on the new proposed model, one can simplify the boundary conditions of this problem. The new boundary conditions are proved to be in line with previous experimental and theoretical results. This paper demonstrates how to proceed normalization and further conversion of the MD simulation results into boundary conditions. Application of the new proposed boundary conditions for Ar–W interactions provides a significant speedup of computations.

1. Introduction

Nowadays a lot of micro/nano systems become an integral part of our daily life, for example: gravity sensor or micro gyroscope are applied in many handheld electronic gadgets. Recent technological advances allowed one to create micro/nano devices with characteristic size of several nanometers. The design processes of such micro/nano devices are very expensive and complicated and involve both experimental and numerical studies of solid and fluid mechanics inside the device. It should be noted that micro/nano flow is characterized by a high degree of rarefaction. It means that assumption of classical continuum theory cannot be applied for analysis of micro/nano flow. Fortunately there is a numerical method, called molecular dynamics (MD) simulation method. It is based on the fundamental principles of mechanics and allows one to simulate processes on molecular level, i.e., the simulated system is considered as ensemble of molecules, rather than a continuous medium.

One of the most challenging parts of numerical simulations of a micro/nano flow is boundary conditions on the solid–liquid interface. The choice of boundary conditions (BC) influences on a flow significantly [1]. The incorrect BC might cause the wrong estimation of fluid behaviors in a micro/nano system. There are two ways to set up the BCs for the MD simulations: (1) to represent the solid parts of the simulated system by molecular structures and consider interactions between fluid molecules and solid boundary molecules; (2) to use relationships which state dependence between parameters of fluid molecule impinged on the solid boundary and the scattered one. The first approach is the most comprehensive one, but one should realize it also increases the number of simulated molecules significantly. Consequently the time of computations rises as well. The second way is widely used due to its relative simplicity. The most commonly used model [1–3] is specular-diffusive model proposed by Maxwell [4] in his studies of gas–surface interactions. The key point of Maxwell's BC is that a gas molecule impinging on a surface is scattered into two fractions, one that reflects specularly and exchanges no energy and the other that accommodates completely and desorbs with an equilibrium distribution corresponding to the surface temperature. Maxwell's BC was extensively used for studies of gas flow through microchannels. Recently we have shown [5] that this specular-diffusive model is too rough to reproduce all the processes accompany the interactions of argon molecules with tungsten substrate.

The energy transfer and other processes accompanying the scattering of rarefied gases from solid surfaces have been the subject of a series of studies. Weinberg and Merrill [6] determined angular distributions for gas atoms scattered by a single-crystal W(1 1 0) surface. The experimental results of Janda et al. [7] allowed the researchers to relate the average kinetic energy of scattered argon atoms to the surface temperature, as well as to the incident kinetic energy. The theoretical explanations for argon atoms scattering from a self-assembled monolayer on Ag(1 1 1) have been proposed recently by Fan and Manson [8]. Furthermore, Gibson et al. [9] conducted a detailed study of Ar scattering from an ordered 1-decanethiol–Au(1 1 1) monolayer. Recently, Chase et al. [16] have conducted experimental and molecular dynamics studies of argon

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scattering from liquid indium. They have shown how the angular and energy distributions of scattered atoms depend on incident energy. Inapplicability of the simple hard-sphere model for the description of gas–surface interactions is also presented.

While there are many publications related to gas–surface interactions, their results are still insufficient to define boundary conditions that can describe the gas flow in micro/nano systems. The best way to study gas–surface interactions is to conduct an experiment, but one should realize that accurate measurements of gas–surface interactions on a microscopic level are very expensive and time consuming. Fortunately, the recent achievements in computer science and numerical methods made it possible to investigate such processes using MD simulation method.

In this paper, MD method was applied to study the argon gas scattering processes on a W(1 1 0) surface. This approach made it possible to precisely describe the interaction between argon gas and tungsten. The aims of this work were to study effects of argon scattering on the tungsten surface and to propose boundary conditions describing correlations between the parameters of incident and scattered atoms. The method applied in the present paper can be simply expressed as the bombardment 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). The combinations of these parameters provide complete information about process of gas atoms scattering process. It is shown that results of current study are in line with experimental and theoretical results obtained by the other researches. The information obtained in simulations was statistically analyzed and represented by polynomial functions of incident energy and angle of incidence. All the functions that state relationship between parameters of impinging gas atoms and scattered atoms have been obtained using the Least Squares Method (LSqM). As a conclusive step of the work, we have proposed an algorithm describing an implementation of the relations mentioned above to a real study of gas flow with tungsten boundary. These relations can be used to specify boundary conditions for argon–tungsten interactions. The main result of this work is proposed new boundary conditions which are able to reproduce mechanism of argon–tungsten interactions and allow one to significantly reduce computation time required for the studies of gas flow around metal surface.

2. Methodology and computation

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

Current research was performed numerically by using MD simulation method. All algorithms described in this study were implemented using Fortran code developed by the authors of this paper. In order to evaluate the gas scattering effects, different collimated beams of argon atoms with intensity of $2{\cdot}10^5$ Pa are set up to impinge on the (1 1 0) face of a tungsten crystal. The interactions among tungsten atoms were taken as being sums of pairwise Morse potential:

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

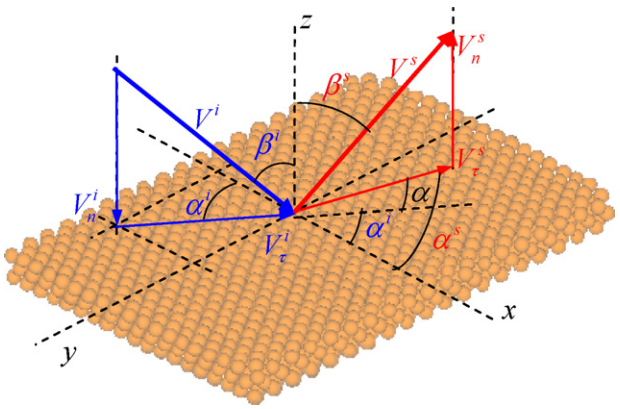

Fig. 1. Coordinate system, where α^i and β^i are the incident azimuthal and polar angles, respectively; α^s and β^s are the scattered atom's azimuthal and polar angles, respectively; $\alpha = \alpha^S - \alpha^i$ are the azimuthal angle change caused by the scattering of gas atom; V^i_n and V^i_τ are the normal and tangential velocity components of the incident atom; V^S_n and V^S_τ are the normal and tangential velocity components of the scattered atom.

where the potential's parameters [10] were: $D_W = 0.9906$ eV, $B_W = 14.116\ nm^{-1}$, $R_W = 0.3032$ nm.

To describe the interaction between both argon–tungsten and argon–argon atoms, Lennard–Jones potential functions are applied and depicted as following:

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

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

where the parameters values used for the case of argon–tungsten and argon–argon, respectively, were: $\varepsilon_{WAr}/k_B = 25.17$ K, $R_{WAr} = 2.93$ Å and $\varepsilon_{Ar}/k_B = 119.18$ K, $R_{Ar} = 3.4$ Å.

The initial lateral position for the impinging atom was selected randomly on a plane 17 Å above the average position of atoms 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. The second order velocity Verlet scheme [10,11] with time step of $\Delta t = 10^{-16}$ s (smaller than the characteristic time of atom interactions) was used for an integration of equations of motion. The computational process was continued until all the gas atoms were within the force field of the tungsten atoms. Scattered gas atoms that went beyond this distance were excluded from the system (argon atoms did not pass through the tungsten substrate), and information on their velocities and coordinates were stored in a file. The exclusion of these scattered atoms reduces the time required for the calculation and prevents the randomization of velocities of argon atoms as a consequence of their collision with each other.

3. Results and discussion

This study was performed for a wide range of initial parameters of the impinging beam and metal surface as well. Total of 1920 cases were computed. The current investigations were conducted for various angles of incidents (from $\beta^i = 0$–70° with 5° steps), a series of surface temperatures ($T_{surf} = 350$ K, 400 K, 450 K, 500 K), and varied velocities of impinging Ar atoms (from $V^i = 100$–1600 m/s with 50 m/s steps).

Any analytical or numerical study based on mathematical descriptions has assumptions and simplifications. Consequently,