



Simulation of the influence of surface chemical composition on internal gas flow at large Knudsen numbers



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ARTICLE INFO

Article history:

Received 25 November 2012
 Received in revised form 5 May 2013
 Accepted 6 May 2013
 Available online 30 May 2013

Keywords:

Gas–surface interaction
 Rarefied gas flow
 Adsorbate
 Auger spectroscopy
 Numerical methods

ABSTRACT

On the basis of the developed model, an attempt to describe a rarefied gas flow in the cylindrical channel, whose surface chemical composition conforms with the real experimental conditions, has been made. During the modeling two cases are considered: the atomically clean silver channel surface and the surface fully covered with the adsorbate, which is simulated by oxygen according to the data of the Auger-spectroscopic analysis. The gas–surface interaction process is based on the molecular dynamic principle. Thermal vibrations of the surface atoms are also considered. The obtained results of calculation are compared with experimental data.

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1. Introduction

When the degree of gas rarefaction increases, the role of interface interaction and the efficiency of heat-and-mass transfer grow considerably as the intermolecular collisions become negligible compared to the molecular collisions with the surface. In the extreme case of the so-called free-molecular regime, the efficiency of heat-and-mass transfer in the “gas–solid body” system is fully determined by the processes occurring on the surface [1].

Until recently, the quantitative estimation of the influence of gas–surface interaction on heat-and-mass transfer represented a considerable problem. Particularly, the reviews containing the experimental data related to the efficiency of heat exchange between a rarefied gas and a solid body provide an extensive field of non-reproducible results [2]. Thus, for example, for the *He–W* systems with similar gas and surface temperatures, different researchers obtain the values of energy accommodation coefficients that have a 20-fold difference (0.02 and 0.4). It means that, depending on the state of the surface, the heat fluxes for such system differ by 20 times in the free-molecular regime. More or less reliable reproducible data were obtained only for clean surfaces prepared according to the special techniques [3], as well as under the conditions that can be implemented on the molecular beam

scattering apparatuses. An impressive result is given in the paper [4], where the removal of surface contaminations results in the tangential momentum accommodation coefficient reaching the minimum value of ~ 0.1 for the *He–Au* system. For a “dirty” surface, the value of the tangential momentum accommodation coefficient is close to 1. Thus, the mass flow for such system in the free-molecular regime can change up to 10 times depending of the state of the surface. It is obvious that the surface condition is of crucial importance in such experiments.

Now the gas–surface interaction problem becomes especially topical due to the development of a new area in the rarefied gas dynamics: Gas Micro Electro Mechanical Systems (GASMEMS). The examples of such systems can include micro-actuators, mass flow and temperature sensors, micro heat-exchangers for electronic component cooling. The fact that the reduction of device dimensions leads to the increase of the Knudsen number $Kn = \lambda/D$ is the key issue that arises in the design process of such devices. Thus, the free-molecular regime is reached at higher gas pressures when the adsorption process becomes of primary importance.

The complexity of theoretical description of gas–surface interaction is connected with the lack of knowledge about the chemical and physical structure of the surface layers. The experimental studies show that the efficiency of energy and mass exchange between a solid surface and gas molecules is affected by multiple factors: these include gas and wall temperatures, gas pressure, type of gas molecules (monoatomic, polyatomic gasses or gas mixtures), chemical composition of the surface (adsorbed layers), as well as the surface roughness. An incident gas molecule can reflect back to the gas phase without exchanging energy with the surface,

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Nomenclature

Kn	Knudsen number, rel. units
D	characteristic length of the system, m
r	radius of the channel, m
l	length of the channel, m
F	interaction force, N
G	relative gas flow rate, rel. units
I	ion current, rel. units
E	energy of electrons, eV
N	intensity of emission of Auger electrons, rel. units number of molecules
L	exposure, 10^{-4} Pa s, relative length, rel. units
T	temperature, K
k	bonding force constant, m^{-1}
M	mass of the atom, kg
W	transmission probability
U	potential
x, y, z	coordinates of particle
X, Y, Z, X', Y', Z'	cartesian axes in physical space
v_m	most probable molecular speed in an equilibrium gas, $m\ s^{-1}$
a	a constant
Δt	integration time interval, s
$Rf()$	random fraction between 0 and 1
P	pressure, Pa
k_b	Boltzmann constant, $k = 1.380658 \cdot 10^{-23}\ J\ K^{-1}$

Greek symbols

λ	mean free path of the molecules, m
θ	surface fraction covered by adsorbed gasses, rel. units
σ	root-mean-square thermal displacement, m^2
μ	molecular weight, a.m.u.
ρ	initial radius, m
η	distribution function
φ, γ, β	angle, grad.
v	particle speed, $m\ s^{-1}$
τ	time interval, s

Subscripts

exp	experimental
$diff$	diffusely, diffuse
g	gas
s	surface
0	initial
gs	gas–surface atomic pair
ga	gas–adsorbate atomic pair
ss	surface–surface atomic pair
sa	surface–adsorbate atomic pair

experience multiple collisions with the surface reaching the equilibrium with it. A particle can also be captured by the surface with the subsequent desorption caused by stochastic processes inside and on the surface of the solid body, or with the formation of a strong chemical bond.

The existing phenomenological structures, such as scattering kernels proposed by Maxwell [5], Cercignani–Lampis [6] and Epstein [7], have a mathematical basis and are artificial to a certain extent. Therefore, each given model has some limitations caused by the complexity of description of the processes occurring at the phase interface. One can make a conclusion that, presently, there is no a multi-purpose scattering kernel fully describing the process of interaction between the gas atoms and the solid body surface. Thus, a more detailed description of interaction requires creation of the models with a greater number of parameters, or movement to a “lower” level of the process description, where the physical and chemical structure of the surface, as well as the interatomic interaction potentials are simulated, using the techniques of molecular dynamics (MD).

Today, due to the growth of the computation power, the simulation based on the MD methods is a powerful tool both for studying individual interactions between gas atoms and a surface and for simulating flows of liquids and gasses in channels. Thus, for example, in the paper [8] the MD method was used for simulating the interaction between a monoatomic gas molecule and the molecules constituting a solid wall in order to study the characteristics of the reflected molecules at the solid surface. Recently, the so-called hybrid methods have become popular [9–12]. Their main idea is to use the MD methods to calculate the interaction of a gas atom with a surface, whereas the motion of gas molecules is simulated using the direct simulation Monte-Carlo. In the above examples of the hybrid methods, a gas particle interacts with surface atoms that are inside the so-called cut-off radius, which size is set based on the parameters of the interaction potential. Thus, the larger the cut-off radius, the more surface particles need to be taken into account when simulating the interaction, and the higher the computation accuracy. On the other hand, the reduction of

the cut-off radius results in the decrease the computation time, but the simulation accuracy in this case notably drops. An example of a more computationally cost-effective method is given in the paper [13], where the vibration potential wall model is proposed. In this model, collisions occur between a particle and a part of a surface assumed as a rigid vibrating body. During the interaction, other particles of the surface are ignored, which allows reducing the computation time.

2. Experimental background

The growth of the processing power and the development of the computer simulation methods, in their turn, allow achieving new results. Particularly, the present paper attempts to describe the rarefied gas flow in a cylindrical channel, whose surface structure and chemical composition conforms to the real experimental conditions [14]. Let us provide a brief description of the experiment. A Pyrex glass cylindrical channel with radius $r = 3.6$ mm and a length $l = 124$ mm ($L = l/r = 34.4$) with a metallic (considered Ti and Ag) filament stretched along the axis is placed in an ultra-high vacuum system. The surface preparation process consists in the deposition of a metal film on the inner channel surface at the residual pressure of about 10^{-10} Pa by heating the respective metal filament. The surface chemical composition is monitored using the Auger-spectroscopic analysis. The mass spectrum of residual gasses of the vacuum chamber (see Fig. 1) and the Auger spectrum derivatives of the channel surface (see Fig. 2) are used to indicate the formation of an adsorbed layer.

Gas flow rate G_{exp} was measured by the technique of efflux from the vacuum chamber at pressure $P_1 = 10^{-8}$ Pa and temperature $T_1 = 300$ K through the capillary into the high-vacuum chamber at pressure $P_2 = 10^{-10}$ Pa and temperature $T_2 = 300$ K.

The measurement results of the relative gas flow rate G of the cylindrical channel in the free-molecular regime for different gasses (He, Ar, Kr) are given in Fig. 3, where the left side of the graph corresponds to the freshly deposited Ti surface and the right side is

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