



**HAL**  
open science

## Temperature, surface roughness and anisotropy effects on the tangential momentum accomodation coefficient between Pt(100) AND Ar

T. Tung Pham, Quy-Dong To, Guy Lauriat, Céline Léonard, V. H. Vo

### ► To cite this version:

T. Tung Pham, Quy-Dong To, Guy Lauriat, Céline Léonard, V. H. Vo. Temperature, surface roughness and anisotropy effects on the tangential momentum accomodation coefficient between Pt(100) AND Ar. 3 rd European Conference on Microfluidics - Microfluidics 2012 - Heidelberg, December 3-5, 2012, Dec 2012, Germany. pp.1. hal-00749274v2

**HAL Id: hal-00749274**

**<https://hal.science/hal-00749274v2>**

Submitted on 21 Nov 2012

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Temperature, surface roughness and anisotropy effects on the Tangential Momentum Accommodation Coefficient between Pt(100) and Ar

Pham T.T., To Q.D.\*, Lauriat G., Léonard C., Vo V.H.

Université Paris-Est, Laboratoire Modélisation et Simulation Multi Echelle, UMR-CNRS 8208,  
5 Boulevard Descartes, 77454 Marne-la-Vallée Cedex 2, France

Department of Physics, Institute of Technology, National University of HochiMinh City,  
268 Ly Thuong Kiet Street, District 10, HochiMinh City-Vietnam

In most applications concerning a fluid flowing past a solid surface, the no-slip conditions are usually employed: the fluid velocity at the wall is assumed to be the same as the surface. This assumption, which works very well in many practical problems, breaks down when the channel height in consideration is at micro/nano length scale. In the framework of the kinetic theory of gases, Maxwell introduced a gas-wall interaction parameter, Tangential Momentum Accommodation Coefficient (TMAC), to quantify the slip effects [1]. He postulated that after collision with the wall, a gas atom rebounds either diffusively or specularly, with the associated portions of TMAC and  $1 - \text{TMAC}$ . Then the slip velocity  $v_{slip}$ , equal to the difference between the gas velocity  $v$  at the wall and the wall velocity  $v_{wall}$ , can be evaluated by the following expression

$$v - v_{wall} = v_{slip}, \quad v_{slip} = \frac{2 - \text{TMAC}}{\text{TMAC}} \lambda \frac{\partial v}{\partial n} \quad (1)$$

where  $\lambda$  is a mean free path and  $\frac{\partial v}{\partial n}$  is the normal derivative of the gas velocity at the wall. Although Molecular Dynamics experiments showed that the reflection mechanism is more complicated than Maxwell's postulation, the coefficient TMAC is still widely used due to its simplicity.

In this paper, we calculated the Tangential Momentum Accommodation Coefficient (TMAC) between Ar and Pt(100) using Molecular Dynamics method (MD). Different from previous work [2], the coefficient is determined directly from the collision based simulation. When the gas is very dilute, this approach proves to be more relevant than simulations of gas flows in slip Navier Stokes regime. The simulation is three dimensional: an Ar atom is projected into a Pt(100) surface with different incident angles  $\theta$  (polar angle) and with different approaching planes  $\varphi$  (azimuthal angle). The TMAC coefficient associated with each  $\theta$  and  $\varphi$  is defined by

the following formula [3]:

$$\text{TMAC}(\theta, \varphi) = \frac{\langle v_{in} \rangle - \langle v_{rn} \rangle}{\langle v_{in} \rangle} \quad (2)$$

where  $v_{in}$  and  $v_{rn}$  are respectively the projections of the incident and the reflected velocity on the vector  $\mathbf{n}$  defining arriving plane. Only one gas-wall collision is treated per simulation and the averages are taken over many simulations (or collisions). The Kulginov potential [4] is used for the couple Ar-Pt while the advanced Quantum Sutton-Chen multi-body potential is employed between the Pt atoms to capture correctly the free surface effect of the walls and atoms trajectory [5, 6]. Different non-flat wall surface models including patterned surfaces, random surfaces and temperature, anisotropy, incident direction effects are studied in this work. Randomly rough surface samples are prepared by separate molecular dynamics simulations of film deposition processes and they are more realistic than mathematical model based [7]. The TMAC result range agrees quite well with the experimental range at the ambient temperature and is not a simply gas-solid constant as proposed initially in the Maxwell model. We also observed that TMAC increase with the roughness of wall and when the temperature decreases. Concerning the anisotropy effect, initial results on systems with stripes show that TMAC varies with orientation.

## References

- [1] Maxwell, J. 1879. On stresses in rarified gases arising from inequalities of temperature. Philos. T. Roy. Soc. A. 170: 231-256.
- [2] To, Q.D., Bercegeay, C., Lauriat, G., Leonard, C. and Bonnet, G. 2010. A slip model for micro/nano gas flows induced by body forces. Microfluid. Nanofluid. 8, 417.
- [3] Karniadakis, G., Beskok, A. and Aluru, N., 2005. Microflows and nanoflows: Fundamentals and simulation. Springer.
- [4] D. Kulginov, M. Persosn, C.T. Rettner, and D.S. Bethune, J. Phys. Chem. **100**, 7919 (1996).
- [5] Sutton, A. P. and Chen, J., 1990. Long-range Finnis-Sinclair potentials. Phil. Mag. Lett. 61, 139-146.
- [6] Subramanian K.R.S.S., Venkat R.B. and Babu J., 2006. Molecular dynamics simulation study of the melting and structural evolution of bimetallic Pd-Pt nanowires. Phys. Rev. B. 74, 155441.
- [7] Majumdar, A. and Bhushan, B., 1990. Role of fractal geometry in roughness characterization and contact mechanics of surfaces. J Tribol-T Asme, 112, 205-216.