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

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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 λ 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 θ (polar angle) and with different approaching planes φ (azimuthal angle). The TMAC coefficient associated with each θ and φ 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.

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