Molecular dynamics study for the friction coefficient between a water droplet and a solid wall

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A fuel cell is an energy device that generates electricity by electro-chemical reaction. Due to its generating mechanism, the theoretical energy translation efficiency of fuel cells is higher than that of heat engines. Especially, polymer electrolyte fuel cell (PEFC) is the most developed one and particular attention is drawn to its progress. This kind of fuel cell can be operated in a relatively low temperature and is expected as the power source for vehicle applications. In PEFC, the electro-chemical reaction occurs at the part called membrane electrode assembly. This assembly is composed of polymer electrolyte membrane, catalyst layers, gas diffusion layers, and micro-porous layers. For stable electro-chemical reaction, water should exist in this assembly to transport protons from anode to cathode. However, at low temperature and high humidity, the gas diffusion layer is obstructed by water generated by chemical reaction, and therefore oxygen gas cannot be supplied to the catalyst layer. This phenomenon is called "flooding". When a micro-porous layer is set between the gas diffusion layer and the catalyst layer, flooding can be controlled, and reactant gas can be supplied stably to the catalyst layer. However, the mechanism is not known in detail. Moreover, owing to the smallness of channel of the micro-porous layer, it is not well-known whether the model based on hydrodynamics can be used. Therefore the behavior of water droplet in micro channel should be analyzed in molecular scale.

In this study, molecular dynamics simulations are performed to evaluate the friction force between a water droplet and a solid wall, and the dependence of the friction coefficient on channel size is clarified. Moreover, we also discuss the limit of hydrodynamic models. From these results, we obtain the basic knowledge about the transport properties of water droplets in the micro-porous layer and the gas diffusion layer.

The macroscopic model of a droplet in a two dimensional planar channel is shown in figure 1a. Considering constant flow, the friction force between a water droplet and a solid wall can be described by a mechanical parameter as

$$F = 2\alpha W_x W_y V_{slip} + 2\sigma(\cos\theta_b - \cos\theta_a) \quad (1)$$

where α is a friction coefficient between a water droplet and a solid surface, W_x and W_y are the contact lengths in x and y direction, θ_a and θ_b are the advancing and receding contact angles, V_{slip} is slip velocity of water on solid walls, σ is surface tension coefficient, respectively[1]. The important point of this equation is the independence of the friction force on the channel width. Based on this equation, to evaluate the dependence of the friction force, we carried out molecular dynamics simulations of different-sized micro channels as shown in figure 1b. This model is composed of two alpha graphite-like slabs with honeycomb structure, and the distance between nearest atoms is 3.0Å. This bond length is determined by adjusting the contact angle of the water droplet on the solid wall. The MPL material used in experiments is highly hydrophobic, and the contact angle is around 145 degree[2]. The macroscopic contact angle derived by the
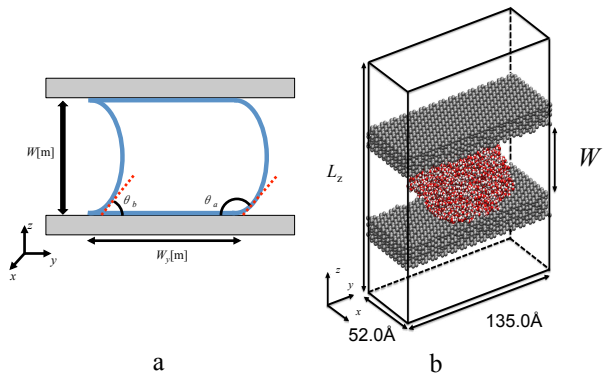

Figure 1. The macroscopic and microscopic channel models. Figure 1a shows the schematic diagram of the macroscopic channel model. Figure 1b shows the simulation model in this study.
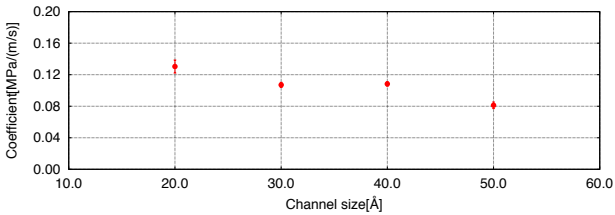

Figure 2. The friction coefficient in eqation (1) as a function of a channel size.

surface tension coefficient between the water droplet and the wall is about 150 degree, which agrees with the experimental value.

Figure 2 shows the friction coefficient, α in equation (1), as a function of a channel size W. According to equation (1), this coefficient is evaluated from the increasing rate of the friction force against contact area. Thus this value means the friction coefficient of water on the region far from the liquid-vapor interface. It can be seen that the friction coefficient decreases with increasing the channel size, while it is a constant in hydrodynamics. This difference is due to the contact pressure generated by the surface tension. When the channel size is in a few nm, the pressure difference between liquid phase and vapor phase by the surface tension is in ten MPa order, since this difference is in a few Pa order in case of an mm channel. In the case of a nm channel, it can be seen that the effect of the surface tension on the region far from the liquid-vapor interface cannot be ignored and strongly affects on the friction coefficient.

Acknowledgement

Reference

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