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PROCEEDINGS

Gas Transport Through Nanochannels: Surface Effect and Molecular Geometry Effect

JianHao Qian[1], HengAn Wu[1] and FengChao Wang[1,*]

[1] CAS Key Laboratory of Mechanical Behavior and Design of Materials, Department of Modern Mechanics, University of Science and Technology of China, Hefei, 230027, China

[*]Corresponding Author: FengChao Wang. Email: wangfc@ustc.edu.cn

ABSTRACT

Gas transport through nanochannels is ubiquitous in nature and also plays an important role in industry. The gas flow in this regime can be described by the Knudsen theory, which assumes that molecules diffusely reflect on the confining walls [1]. However, with the emergence of low dimensional carbon-based materials such as graphene and carbon nanotubes, it has been evidenced that this assumption might not hold for some atomically smooth surfaces, resulting in an anomalous enhancement of gas flux [2]. Moreover, in Knudsen theory, gas molecules are usually treated as mass points and distinguished solely by molecular weight, which cannot interpret recent experiments that gases with similar molecular weight exhibit a remarkable difference in the flow rate [3]. In this talk, I will present our recent research progress in this field. We meticulously investigated the gas transport through nanochannels. For the enhancement of gas flux through nanochannels with atomically smooth walls, we revealed the underlying mechanism as the surface morphological effect on the gas collision with solid walls [4]. Even a subtle distinction of surface roughness results in specular scattering on graphene surfaces while diffuse scattering on molybdenum disulfide surfaces. We found that the curvature effect could reduce the surface roughness of interaction potential surfaces, leading to an additional enhancement on the gas flow rate. We also ascertain the molecular geometry effect on the transport of various gases through nanochannels [5]. Gas molecules with a complex geometry are more likely to experience multiple reflections on the surface, leading to the diffuse scattering and a reduced flux. During the collision, only the normal translational kinetic energy acts as a positive contribution to the successful reflection, while the vibrational, rotational and tangential translational kinetic energies are all ineffective in this process. The ratio of this ineffective energy to the initial kinetic energy is suggested as the criterion whether the gas can disengage from the wall after each collision. These insights are expected to deepen the understanding of gas transport in nanochannels, paving a promising way in the gas permeation control. Our work also offers a new perspective to extend Knudsen theory for broader applications.

KEYWORDS

Gas transport; nanochannels; Knudsen theory; surface morphological effects; molecular geometry effect

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