

Topical Review

Atomistic simulations of the frictional properties of 2D materials: a review

Gang Wu¹, Shigenobu Ogata^{2,*}  and Lei Gao^{1,2,*} 

¹ Beijing Advanced Innovation Center for Materials Genome Engineering, Institute for Advanced Materials and Technology, University of Science and Technology Beijing, Beijing 100083, People's Republic of China

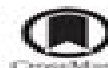
² Department of Mechanical Science and Bioengineering, Osaka University, Osaka 560-8531, Japan

E-mail: ogata@me.es.osaka-u.ac.jp and gaolei@ustb.edu.cn

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Abstract

The two-dimensional (2D) materials are regarded as the ideal solid lubricants at micro- and nano-scale. Besides the experiments and analytical models, the atomistic simulations are important tools to investigate the frictional properties of 2D materials. This review will focus the recent atomistic simulation studies on frictional properties 2D materials with a particular emphasis on the density functional theory (DFT) calculations and molecular dynamics (MD) simulations. Starting from the proper calculation of long range dispersion forces, the correlations between the physical characteristics (e.g. electronic charge redistribution, interfacial commensurability, chemical modification, moiré superlattice, layer effect, atomic contact quality, defect, external fields, humidity and temperature) and frictional properties of 2D materials are reviewed for both the interlayer and surface sliding. Meanwhile, recent MD simulations about the phononic energy dissipation in friction of 2D materials are summarized. At last, some shortcomings in current simulation techniques are summarized and it is suggested that the atomistic simulations combined with machine learning will be a more powerful strategy to investigate the frictional properties of 2D materials.

Keywords: atomistic simulations, 2D materials, friction, density functional theory, molecular dynamics simulation

1. Introduction

To tune and reduce the friction and energy loss is desirable for the mechanical systems with moving parts at all length scales, especially at nano-scale, where large ratios of atoms reside at the surface and interface sites [1]. To achieve the goal of reducing friction and mitigating wear, it calls for the finding of origin of friction from the atomic scale. Recently, superlubricity, a state of vanishing friction has drawn intensive attentions and been well investigated by experiments and atomistic simulations [2–5]. More specially, structural superlubricity

between the crystalline surfaces is regarded an approach to achieve superlubricity in real industrial applications [6]. Motohisa Hirano proposed that superlubricity appears when the system satisfies two conditions: each atom follows its equilibrium position adiabatically, and the contacting crystal surfaces are incommensurate [7].

Two-dimensional (2D) layered materials such as graphene, hexagonal boron nitride (h-BN), and molybdenum disulfide (MoS₂) have attracted great scientific and technological interests due to their unique electronic [8, 9], mechanical [10, 11], and frictional properties [12–16]. The discovery of 2D materials provides an ideal and abundant pool to form the incommensurate interfaces that might possess superlubricity property and it is supposed as an important approach to

* Authors to whom any correspondence should be addressed.

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