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Anisotropic nanoscale and sub-nanoscale friction behaviors between phosphorene and silicon tip

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ABSTRACT

Understanding the frictional properties of phosphorene is essential for reliable fabrication and sustainable operation of phosphorene-based nanotechnology devices. Although recent studies have revealed that phosphorene exhibits anisotropic frictional characteristics, the detailed mechanisms are not well analyzed, and the influence of some experimental parameters (e.g., spring stiffness, tip load force, and tip size), which are very sensitive to atomic frictional forces, were not considered. This study was carried out to address the above shortcomings. The anisotropic frictional behavior of phosphorene and its detailed mechanism were analyzed using potential energy profiles. Also, the effects of spring stiffness and tip load force on the stick-slip behaviors were investigated. Furthermore, we studied the sub-nanoscale stick-slip behavior during the nanoscale slip motion. The nanoscale and sub-nanoscale stick-slip phenomena were originated from the tip's behavior of passing over the bond between the phosphorus atoms and over the puckered honeycomb structure along the zigzag and armchair directions. We utilized a simple one-dimensional model to explain the energy profiles. The influence of tip size on the stick-slip behavior was also examined and found related to the initial nanoscale slip velocity. As the tip diameter decreased, a high-frequency sub-nanoscale stick-slip phenomenon and shorter nanoscale slip duration were identified.

1. Introduction

Phosphorene is an allotrope of phosphorus which refers to a single-layer of black phosphorus. Compared to graphene with a band gap of 0 eV [1,2], phosphorene has a band gap of 1.5 eV [3] and a high on/off ratio of 10^4 [4]. It also has higher electron mobility ($\sim 10,000 \text{ cm}^2/(\text{V}\cdot\text{s})$) [3] than transition metal dichalcogenides (TMDs) ($\sim 500 \text{ cm}^2/(\text{V}\cdot\text{s})$) [5]. Therefore, phosphorene is a material with a high electric control capability and has a wide application range as an optical and photoelectric device [6–8]. Also, due to the unique puckered honeycomb structure, it exhibits anisotropic mechanical properties of the Young's modulus and deformability [9,10]. When applying the mechanical strain on phosphorene, the strain-induced lattice shift of the phosphorus atoms affects the band structure, and hence the electronic and optical properties of phosphorene [11–15].

Because of these remarkable features, phosphorene has been used in numerous studies on strain engineering nanotechnology to meet certain requirements of phosphorene-based applications [16–18]. Due to the large surface-area-to-volume ratio of these nanoscale devices, the effect of surface forces (e.g., friction, stiction, and wear of the small contacts)

on the elements that are in relative motion has become a major technological topic [19,20]. These tribological phenomena restrict the smooth operation of the devices and thus are the dominant degradation mechanisms noticed in nanotechnology devices [21]. Therefore, it is fundamental to explore the tribological mechanisms of phosphorene for the reliable fabrication and sustainable operation of phosphorene-based nanotechnology devices.

To study the tribological properties of two-dimensional materials, previous studies have used friction force microscopy (FFM) [22–24]. With this experimental tool, fundamental insights into relevant processes have been gained on various two-dimensional materials at nanoscales [25,26]. Recently, both FFM experiment and simulation model confirmed the anisotropic frictional characteristics of phosphorene [27,28]. More specifically, these studies observed the higher friction forces in the armchair direction more closely than in the zigzag direction. However, a systematic study of the type of frictional mechanisms on the interface between the FFM tip and the phosphorene that provokes the anisotropy has yet to be carried out. In addition, although atomic friction is very sensitive to a variety of experimental conditions including spring stiffness, FFM tip load force and size, at present, there

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