Tribology International 77 (2014) 211–217

Contents lists available at ScienceDirect

Tribology International

journal homepage: www.elsevier.com/locate/triboint

Effect of strain on atomic-scale friction in layered MoS_2

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ARTICLE INFO

Article history:
Received 29 November 2013
Received in revised form
13 February 2014
Accepted 20 February 2014
Available online 27 February 2014

Keywords:
First-principles
Friction
MoS_2
Strain

ABSTRACT

The atomic-scale friction in MoS_2 is investigated employing the density functional theory calculation including the dispersion correction (DFT-D). Energy corrugations and lateral frictional forces of the lamellar MoS_2 are derived, suggesting that the in-plane compressive MoS_2 exhibits lower friction than the tensile system. The reduced friction is attributed to a stronger coulombic repulsive interaction enabled by the transferred charge to the sliding interface. In-depth understanding of the relationship between friction and interfacial interaction shows that friction can be tuned in layered MoS_2 by applying an in-plane strain to the sliding interface.

1. Introduction

The development of nano-materials highlights the need to understand how such materials behave in relative sliding friction process. The understanding of atomic-scale friction is important to deeply investigate the mechanisms of wear, energy dissipation and lubrication for data storage devices, coatings, composites, and eletro-mechanical systems in nano-scale. The two-dimensional (2D) material, single-layer MoS_2, has attracted extensive study for potential applications in nanoelectronics mainly owing to its exotic physical properties [1,2]. This motivates the development of the monolayer MoS_2 for next-generation electronic devices and nano-eletro-mechanical systems [3,4]. For such applications, the mechanical and tribological properties of this material must be better understood. Although it is generally recognized that the excellent lubrication of MoS_2 sheets is based on its lamellar structure, the detailed chemical and physical interactions between layers are still unclear in the friction process.

Hexagonal MoS_2 with a honeycomb structure is a lamellar compound used for a long time as a solid lubricant because of its excellent performance as a friction reducer [4–6]. Bulk MoS_2 is a indirect semiconductor with a bandgap of 1.23 eV [7]. In experiment, when the crystal is mechanically exfoliated to monolayer, MoS_2 emerges a direct semiconductor with a gap of 1.80 eV [1]. Recently, its bandgap can be continuously tuned from direct to indirect or from semiconducting to metallic properties by applying mechanical strains identified as one of the best possible strategies to tune the bandgap [8–12]. Strain can result from externally applied stress, or when a 2D material is clamped to a substrate [13]. The presence of strain in low-dimensional materials can have profound effects upon many properties, and hence it is important to understand nanoelectronic devices, nanocoatings, nanocomposites, and nanoeletromechanical systems. The friction between atomically smooth surfaces in these systems is dominated by the atomic structures and interatomic interactions at the sliding interface. And hence electronic structure at the interface plays an important role on the interaction. An in-depth understanding of the relationship between atomic-scale friction and interfacial interactions reveals that the friction can be tuned by structural and chemical modifications to the sliding surfaces [14–17]. This motivates us to change the interfacial interactions and then tune the interlayer friction by applying biaxial in-plane strains to the layered MoS_2.

In this paper, for the purpose of better understanding the frictional behaviors between MoS_2 layers, particularly the effect of in-plane strains, we investigate its influence on the interlayer sliding using density functional theory (DFT) calculations including van der Waals (vdW) correction. Previously, Onodera et al. [5] have studied the atomic interactions between MoS_2 sheets by using a hybrid quantum chemical/classical molecular dynamics method. They found that the predominant interaction between two sulfur layers in different MoS_2 sheets was Coulombic repulsion, which directly affects the MoS_2 lubrication. Moreover, this group investigated the friction anisotropy of two-layered MoS_2 at atomistic level using the same method [6]. Their results showed

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http://dx.doi.org/10.1016/j.triboint.2014.02.013
0301-679X

that lubrication by MoS_2 strongly depended on its interlayer contacts in the atomic scale and the rotational disorder was also important to achieve low friction state. Blumberg et al. [18] provided a simple and intuitive explanation for the interlayer sliding energy landscape of MoS_2 on the basis of the registry index (RI) concept. Quantum mechanics based first-principles methods are widely recognized as a powerful tool to examine the nature and consequences of the interactions between surfaces at the nano-scale. Using the local density approximation (LDA) pseudo-potentials calculations, T. Liang et al. [14] have calculated the static potential energy surface of MoS_2(001) and MoO_3(001) surfaces and of the MoO_3(001)/MoS_2(001) interface under pressures of 500 MPa applied normal to the sliding interface. Their results indicated that it was the easiest to move MoO_3 over MoS_2 along the channel direction formed by S atoms at the sliding surface and the hardest for MoO_3(001) interlayer sliding. Moreover, within the generalized gradient approximation (GGA) calculations including van der Waals corrections, the frictional figure of merit for a pair of layered MoS_2 nanostructures has been determined by Cahangirov et al. [19]. They showed that the layered structure had low critical stiffness even under high loading forces due to their charged surfaces repelling each other. The intrinsic stiffness of the material exceeds critical stiffness and thereby the material avoided the stick-slip regime and attains nearly dissipationless continuous sliding. However, all the above researches have not considered the effect of in-plane strains. In-depth understanding of the relationship between atomic-scale friction and interfacial interaction indicates that the interlayer friction in MoS_2 can be tuned by mechanical strains. These investigations may be helpful for friction control, as well as electronic device and lubricant design.

2. Details of calculation methods

The First-principles calculation within DFT is widely considered as a powerful tool for examining interatomic interactions and predicting electronic structures. However, the popularly employed local density approximation (LDA) and generalized gradient approximation (GGA) for the exchange correlation functional are unable to well describe the dispersive interaction (vdW interaction), which is thought to control the structure of proteins, the packing of crystals, or the orientation of molecules on surfaces [20]. In the MoS_2 system, vdW dispersive and electrostatic interactions dominate and determine the interlayer or interfacial structures and properties. The van der Waals density functional (vdW-DF) [35,36] is a non-local correlation functional that approximately accounts for dispersion interactions. Several proposed versions of the method can be used: the original vdW-DF [36], the "opt" functionals (optPBE-vdW, optB88-vdW, and optB86b-vdW) where the exchange functionals were optimized for the correlation part [21], and the vdW-DF2 [37]. In this paper, a more accurate exchange functional, recently derived by Klimeš [21,22], for long-range dispersive interaction is included in our DFT calculations.

In our calculations, DFT implemented in the Vienna Ab-initio Simulation Package (VASP) [23,24], is employed to calculate electronic structures and total energy. The exchange-correlation functional is represented with the GGA in the form of the Perdew–Burke–Ernzerhof (PBE) [25]. The interaction of valence electrons with atomic cores is described using the projector-augmented wave (PAW) method [26,27], and the electronic wave functions are expanded in a plane-wave basis with the energy cutoff of 500 eV to converge the relevant quantities. Total energy and electronic structures of the systems with different in-plane strains are calculated using a $15\times15\times1$ Monkhorst-Pack (MP) grid [28]. The convergence for energy is chosen to be 10^{-5} eV between two electronic relaxation steps, and the maximum force allowed on each atom is less than 10^{-2} eV/Å upon ionic relaxation.

A (1×1) supercell used in the present study consists of two layers of MoS_2 sheets to simulate their relative sliding. As shown in Fig. 1, we expand the (1×1) supercell to (3×3) for convenience. Biaxial in-plane strain has been applied by imposing a value of the in-plane lattice parameters $\boldsymbol{a}$, corresponding to a strain $\varepsilon=\frac{a-a_0}{a_0}\times100\%$. a_0 is the lattice constant in the state of equilibrium. Positive and negative signs represent tensile and compressive strains, respectively. Seven models with different in-plane strains ($\varepsilon=-18\%$, -15%, -10%, 0%, $+5\%$, $+10\%$ and $+15\%$) are built to investigate the deformed effects on interlayer friction. To eliminate the interactions between adjacent supercells, we consider the computional supercell with a length of 30 Å in the z direction, leaving a vacuum region of more than 20 Å. For each value of x along the sliding direction, the fixed atomic layer at the top is displaced manually along z direction. At each mesh point, except those of fixed top and bottom planes, all atoms of the system are relaxed using the conjugate gradient method [29]. The loading method is the same as that in previous works [19,38]. In order to study the load effect on the friction along the considered path (x direction as shown in Fig. 1), we investigate the variation of the system energy corrugation (the difference between the maximum and minimum energies) and the maximum static lateral force under different loads. The top S atom in the upper MoS_2 layer and the bottom S atom in the lower layer are constrained, while other atoms are free when calculations are carried out under a series of given interlayer distances or different displacement along the path. Thus the system energy at each mesh point can be obtained, and then the normal load and the lateral friction force can be derived. Eventually, the matrices of all data are spline interpolated. Therefore, the variation of system energy and static lateral force can be derived as one layer slides along the path under a given constant load. And the interaction energy of the system described elsewhere [15–17] is calculated to be $E_i=E_t-2E_s$, where E_t is the energy of the supercell containing two MoS_2 layers and E_s is the energy of a single layer with the same in-plane strain. During the sliding process along the x direction, there are four high

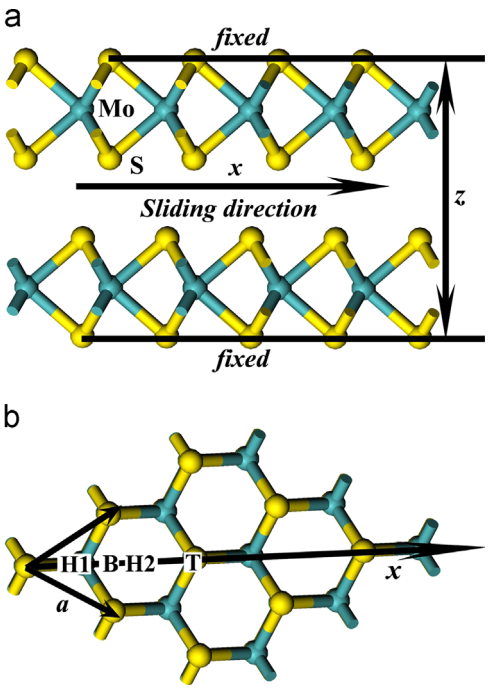

Fig. 1. Ball and stick model of MoS_2 used in the present study. Yellow and aqua balls represent S and Mo atoms, respectively. (a) side view (b) top view.