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Spin friction between Co monolayer and Mn/W(110) surface: *Ab Initio* investigations

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ABSTRACT

Employing first-principles approach within density functional theory (DFT), spin friction properties of Co monolayer sliding on Mn/W(110) substrate were investigated (Wolter et al., 2012) [22]. The magnitude of spin friction is obtained by calculating the friction difference between the spin-polarized and non-spin-polarized cases. Our results reveal that the magnetic system exhibits significantly lower friction than the non-magnetic system, which can be explained by an electronic level mechanism of spins on friction properties. Additionally, this study provides an approach to estimate the spin friction under the formwork of DFT.

1. Introduction

Friction plays an indispensible role in people's life, and studies on friction are also time-honored. With the development of tribology, it has been known that friction can be reasonably and effectively controlled until correctly understanding its microscopic mechanisms [1]. At atomic scale, a micro system moving on one surface induces lattice vibrations producing phonons associated with energy dissipation near the interface, and simultaneously stimulates conduction electrons generating electron–hole pairs dissipating energy, in which these two ways are known as phononic friction [2–5] and electronic friction [6], respectively. Electronic and phononic frictions have been investigated extremely for a long time, and significant conclusions have been reached [7–12]. Electronic friction is the main dissipative channel in the metallic state, while phononic friction dominates in the superconducting state. Since electronic friction dissipates energy via excitation of low-energy electron–hole pairs mainly in the interface of metals, spins as an intrinsic property of electrons must dissipate energy if they change or flip during the motion of magnetic friction system. The friction induced by spins is called spin friction, which has been recently advanced as a new mechanism of friction [13,14].

With extensive applications of magnetic materials and developments of advanced experimental methods, such as magnetic force microscopy (MFM) and spin polarized scanning tunneling microscope (SP-STM), spin friction has attracted increasing interests recently [15–19]. Theoretically, within the framework of classical Heisenberg-model, Fusco et al. demonstrated that the motion of magnetic tip with respect to the magnetic surface could lead to the creation of spin waves which dissipate energy [14]; based on the stochastic Landau–Lifshitz–Gilbert equation, Magiera et al. investigated the spin excitation mode of energy dissipation in a moving magnetic tip interacting with surface [20,21]. However, these studies cannot reveal the role of spins in nanofriction for lack of experimental supports. Recently, Wolter et al. studied the spin friction of one cobalt (Co) atom on Mn/W(110) surface by SP-STM experiment combined with Monte Carlo simulations [22]. They found that the average friction force spans a wide range (−50% to 60%) with the enhancement of tip–adatom exchange interaction after introducing the spin degrees of freedom. This work illustrated the friction differences between non-magnetic and magnetic systems, which confirmed the importance of spins in nanofriction for magnetic materials. But it needs to be assisted by a magnetic tip, and constantly changing the strength of tip–adatom exchange interaction, and also not directly obtaining the magnetic moment variation of every magnetic atom in sliding process.

The development of computational capabilities has greatly promoted the theoretical simulations of friction, and the

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commonly used method is molecular dynamics (MD) simulations. However, classical MD simulations are too dependent on the empirical potentials, and also cannot deal with the quantum systems with spins. In contrast, the first-principles based on DFT is a more accurate method calculating electronic structure and hence nanofriction, which has been applied to many systems [23–32] since proposed by Zhong et al. [33–35]. In this paper, we firstly employed DFT to study the contribution of spin degrees of freedom to nanofriction. For comparison with the reference [22], we also chose an antiferromagnetic (AFM) Mn monolayer on bilayer W(110) as substrate, on which a magnetic Co monolayer is adsorbed to form a simple research model. Our calculations showed that the friction of magnetic system is obviously lower than that of non-magnetic system, fully illustrating the role of spins in nanofriction for magnetic materials. Our results are in good agreement with those of Wolter et al. [22]. Furthermore, spin frictions and magnetic moments of atoms during sliding can be directly obtained in our calculations.

2. Computational methods

Besides the phononic friction, the friction can be caused by electrons and spins, namely electronic friction and spin friction. In our model, we only considered the friction contributed by electrons, together with their spins, defining the spin friction owing to the spin interactions for magnetic materials in this way,

$$f_{\text{spins}} = f_{\text{mag}} - f_{\text{non-mag}} \tag{1}$$

where f_{mag} and $f_{\text{non-mag}}$ are the frictions of magnetic materials considering spins or not, respectively. Eq. (1) indicates that the spin friction f_{spins} is the difference between the magnetic system and the corresponding non-magnetic system. In this paper, we could roughly estimate the magnitude of spin friction according to the above formula by calculating f_{mag} and $f_{\text{non-mag}}$.

All the calculations were performed using the Vienna Ab-initio Simulation Package (VASP) code [36,37], equipped with the projector augmented-wave (PAW) method for electron–ion interaction [38,39]. The exchange–correlation interaction was treated with the generalized gradient approximation (GGA) in the parameterization of Perdew–Burke–Ernzerhof (PBE) [40]. The wave functions were expanded in a plane-wave basis with an energy cutoff of 500 eV. A 2×2 supercell of Mn/W(110) was chosen to simulate the friction surface and Co monolayer sliding on it, which is a periodic structure. A vacuum layer at least 15 Å was set to avoid the interaction between adjacent images. The irreducible Brillouin zone integration was carried out by using $11\times11\times1$ Monkhorst-Pack grids for our model [41]. The total energy was converged up to 10^{-4} eV for electronic structure relaxations. For geometry optimizations, all the internal coordinates were relaxed until the Hellmann–Feynman forces were less than 0.02 eV/Å. We analyzed the magnetic and non-magnetic systems using the spin-polarized (SP) and non-spin-polarized (NSP) calculating results, respectively.

The Mn/W(110) substrate (Fig. 1(a)) was optimized by relaxing only the z direction of Mn atoms in the topmost layer and fixing the two bottommost W layers in their bulk positions. Subsequently, the model was constructed by dragging one Co adatom over the relaxed Mn/W (110) substrate (Fig. 1(b)), three highly symmetrical sliding paths selected (Fig. 1(c)), namely path I, II and III, which correspond to [001], $[1\bar{1}0]$ and $[\bar{1}1\bar{1}]$ directions in bulk bcc Mn, respectively. Such three highly symmetrical paths cover all the special stacks in the Mn/W(110) surface, and the other paths can be combined by them. For convenience, four Mn atoms in 2×2 supercell are labeled as Mn1, Mn2, Mn3 and Mn4, whose locations in the surface are appropriately four top positions called T1, T2, T3 and T4, respectively. The intersection point of path I and path II is the hollow site of surface abbreviated to H, and the midpoint of path III is one of bridge sites in surface called B.

To estimate the magnitude of spin friction, frictional properties for both magnetic and non-magnetic systems were calculated. It should be noticed that the four Mn atoms are identical in the non-magnetic system but nonequivalent in the magnetic one due to the AFM spin distributions. The spin direction of Mn1 and Mn3 (spin down) is antiparallel with that of Mn2 and Mn4 (spin up). To find out the barrier of each sliding path, the sliding processes were modeled through moving Co atom from initial position to final position in 10 steps of 0.274 Å each in path III, and in 8 steps of 0.198 Å and 0.280 Å each in path I and II, respectively.

3. Results and discussion

3.1. Interaction energies

Atomic-scale friction properties are closely related to the interacting energy of two bodies with relative sliding. The interaction between Co monolayer and Mn/W(110) surface is mainly expressed by adsorption energy (E_{ad}), which was calculated by

$$E_{\text{ad}}(z) = E_{\text{total}}(z) - E_{\text{Mn/W(110)}} - E_{\text{Co}} \tag{2}$$

where E_{total} is the total energy of system, and $E_{\text{Mn/W(110)}}$ (E_{Co}) is the energy of Mn/W (110) substrate (Co monolayer). The distance z is the adsorption height of Co on surface along z axis.

The energy was calculated when the Co monolayer and the substrate were brought together with a decrement of 0.05 Å from the adsorption height of 2.60 Å. In the calculation of the E_{total}, all of the atoms were fixed, and only the distance between Co monolayer and Mn/W(110) surface was changed. This is different from the method proposed by Wolloch et al. that energy is dissipated via the relaxations in the sliding materials themselves [42]. The adsorption energies as a function of adsorption heights in different stacking

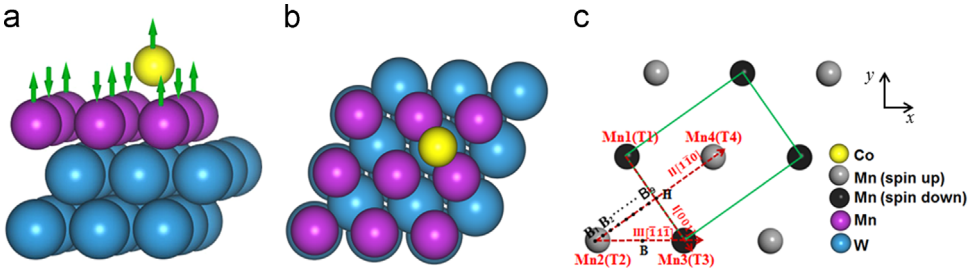

Fig. 1. (a) side view and (b) top view of the calculated model, in which a Co atom slides on the surface of a 2×2 Mn/W(110) surface, and the spin directions of Mn atoms are arrayed in AFM order. The green arrows represent spin directions of Co and Mn atoms. (c) the Schematic diagram of three sliding paths. The rectangle denotes one magnetic unit. Gray and black balls show spin up and spin down of Mn atoms, respectively. The different configurations are shown with B1–B9 in sequential order along path II. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)