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Electronic and transmission properties of magnetotunnel junctions of cobalt/iron intercalated bilayer two dimensional sheets

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ABSTRACT

Density functional theory and the nonequilibrium Green's function method are used to study the electronic properties and tunneling magnetoresistance (TMR) of magnetotunnel junctions (MTJs) based on Co/Fe intercalated bilayer graphene (bi-Gr), bilayer hexagonal boron nitride (bi-h-BN), and bilayer Gr-h-BN (bi-GBN). The spin-polarized bands around the Fermi energy of the two dimensional bilayer sheets are modulated by the intercalated cobalt. The TMR ratio reaches 169.94% and 173.00% for cobalt and iron intercalated Ni|bi-GBN|Ni MTJs, respectively. We observe that the Co/Fe intercalated bi-GBN is a promising candidate as a spacer in MTJs for spintronics.

1. Introduction

Graphene (Gr), a single layer of carbon atoms, has attracted attention owing to its peculiar electronic characteristics [1–3] and potential for application in spintronics [4–6]. One of the fundamentals of spintronics is spin filtering, which involves the tunneling magnetoresistance (TMR) effect in magnetotunnel junctions (MTJs). Such spin filters are achieved by electron transmission selectivity of the interface between the insulator (or semiconductor) and ferromagnetic metal (FM) [7,8]. The TMR ratio is the most important parameter of MTJs [9,10], which is a crucial factor for many technological applications, such as magnetic random access memory applications, sensors, and logic circuits [7,8]. However, the difficulty of obtaining well-ordered interfaces is the main obstacle in achieving a high TMR ratio [11–13]. Recently, using multilayer graphene or h-BN as a spacer, a relatively high TMR ratio was achieved both in experiment and theory [14–16]. The results indicate that graphene and h-BN are promising candidates for the spacer in MTJs.

Graphene and h-BN can be directly grown on a variety of transition metal substrates by the chemical vapor deposition (CVD) method [17–21]. The covalent bond of graphene and the h-BN sheet is perfectly preserved on the substrates, and the quality of the interface between the transition metal and such layered materials is perfect owing to the small lattice mismatch [22–25]. For example, the mismatch between Ni(111) and graphene or h-BN is less than 2%. The well-ordered interface between graphene/h-BN and a transition metal is attractive as the spacer of MTJs. Previous theoretical investigations [14–16,26] have reported that the MTJs based on graphene and h-BN can achieve high spin filtering and TMR ratio. Further studies have found that the interface roughness [15], heterogeneous interface [16,27], external uniaxial strain [28], and external electric field [29] are all important factors to realize high spin filtering and TMR ratio. The TMR ratio for MTJs is determined by the matching of the spin dependent transport channels between electrodes and spacer, especially the spin-dependent transport states of the spacer around the Fermi energy. In a previous study [28], we increased the TMR ratio of the Ni|BN-BN|Ni MTJs through modulating the electronic structures of the bilayer BN sheet by uniaxial strain. Recent theoretical results [30] indicate that transition metal (including Fe, Co) intercalation can strongly modulate the structural, electronic, and magnetic properties of bilayer 2D sheets, including bilayer graphene, bilayer-graphene/hexagonal-boron-nitride, and bilayer hexagonal boron nitride. Especially, Co/Fe intercalation induces spin-polarization around the Fermi level of the bilayer systems. Such spin-polarization around the Fermi level is suitable for the spacer of the MTJs. The transition metal intercalation provides another approach to enhance the TMR of the MTJs composed from bilayer systems. Using density functional theory, we find that the bands around the Fermi energy of the two dimensional bilayer

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sheets, including bilayer graphene (bi-Gr), bilayer hexagonal boron nitride (bi-h-BN), and bilayer Gr-h-BN (bi-GBN), are severely modulated by the intercalated cobalt or iron. Interestingly, the TMR ratio of the MTJs based on Co/Fe intercalated bilayer systems is in excess of 100%, which is close to the value observed for a perfect spin filter.

2. Computational methods and models

We use two semi-infinite Ni(111) electrodes and Co/Fe intercalated bi-Gr, bi-h-BN, and bi-GBN as the spacer to construct the MTJs, as shown in Fig. 1. The in-plane lattice constants of bi-Gr, bi-h-BN, and bi-GBN match well with the surface lattice constant of Ni(111). Moreover, this choice of electrodes is convenient for comparing the results in our present work with previous theoretical [14–16] and experimental [31,32] reports. To obtain the electronic and stable structures of MTJs, we adopt the Vienna ab initio simulation package (VASP) [33,34] to perform the first-principles plane-wave calculations within the density functional theory (DFT). We choose the local density approximation (LDA) [35] as the exchange-correlation functional. A plane wave basis set with a kinetic energy cutoff of 450 eV was employed. The Brillouin zone was sampled by $7 \times 7 \times 3\Gamma$-centered Monkhorst–Pack grids. Crystal lattices and atom positions of all systems are fully optimized up to the residual force on every atom less than 0.02 eV/Å through the conjugated-gradient algorithm; and the total energies are converged to 10^{-5} eV. Using the nonequilibrium Green's function based on first-principles method, the transport calculations are carried out using the Atomistix ToolKit (ATK) package [36]. The single and double ζ plus polarization numerical orbitals for Ni and B(C,N) atoms, respectively, are used in place of the plane wave basis set. The exchange and correlation potential is approximated by LDA [35,37]. The total energy is converged to 10^{-5} Ry and the energy cutoff is set to be 300 Ry. A $30 \times 30 \times 100$ Monkhorst–Pack grid is used in the Brillouin zone. The TMR ratio is defined as:

$$TMR = \frac{G_P - G_{AP}}{G_{AP}} \times 100\% \tag{1}$$

where G_P and G_{AP} are the transmission conductance in the parallel (P) and the antiparallel (AP) configuration, respectively.

3. Results and discussions

There are three possible configurations when Gr is added on the Ni(111) surface. The most favorable configuration is that half of the carbon atoms are located above the interface nickel atoms, while the others are located on the fcc hollow sites [38,39] (such a configuration is termed top-fcc), as shown in Fig. 1(a). Cobalt and iron intercalated bi-Gr with AB and AA stacking shows a similar binding energy [30]. To enable comparison with a previous report, we chose the Co/Fe intercalated AA stacking bi-Gr as a typical model. Fig. 1(c) shows the cobalt intercalated AA stacking bi-Gr sandwiched by the two semi-infinite Ni(111) electrodes. The models are denoted as Ni|Gr-Co-Gr|Ni and Ni|Gr-Fe-Gr|Ni. We have previously observed that the most stable configuration of Ni|bi-BN|Ni MTJs is AA stacking with N atoms sitting atop the nearest layer Ni atoms and B atoms located on the third neighboring layer Ni atoms [28]. Thus, AA stacking of bi-BN is used as the cobalt intercalated system and the optimized configuration for the system is shown in Fig. 1(g). The systems are denoted as Ni|BN-Co-BN|Ni and Ni|BN-Fe-BN|Ni. Considering both adsorption configurations of Gr and h-BN on the Ni(111) surface, the most stable configuration of cobalt intercalated bi-GBN is shown in Fig. 1(e), which are named as Ni|Gr-Co-BN|Ni and Ni|Gr-Fe-BN|Ni. To study the effect of cobalt and iron on the spin filtering, we use Ni|Gr-Gr|Ni, Ni|BN-BN|Ni, and Ni|Gr-BN|Ni as systems for comparison, as shown in Fig. 1(b),

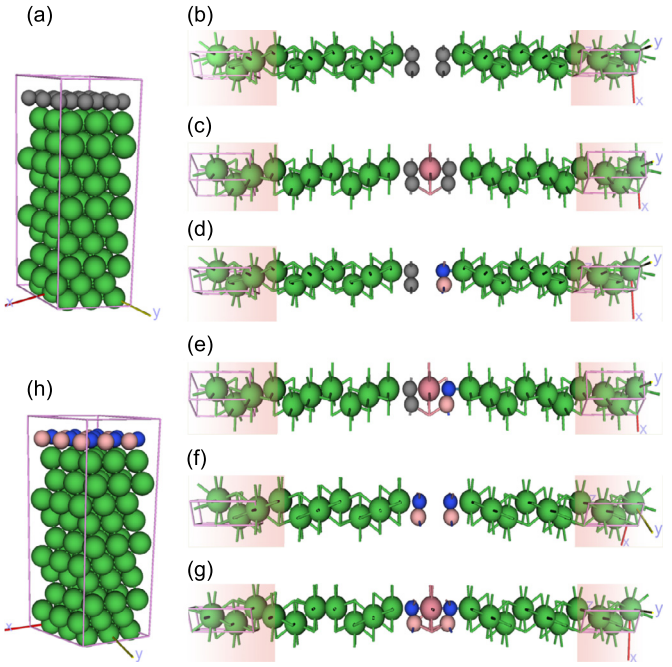

Fig. 1. (a) and (h) are schemes of the Graphene and h-BN adsorbed on Ni(111) surface, respectively. (b)–(g) are side views of the three types of bilayer sheet sandwiched between two semi-infinite Ni(111) electrodes with and without cobalt intercalated, respectively. Carbon, Nickel, Born, Nitrogen, and Cobalt atoms are represented by gray, green, pink, blue, and hot pink spheres, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 1(f), and Fig. 1(d), respectively. The relative position of the interface between Ni(111) and Gr (h-BN) in our present work agrees well with previous reports [15,26,28]. We find that the bond length of Ni–C(Ni–N) is about 2.3 ∼ 2.0 Å, and the C–TM (N–TM) is about 2.1 ∼ 2.0 Å. All the parameters for the optimized structures are shown in Table 1 and Table S1 in the Supporting Information. The distance of the inter-layer of bi-Gr, bi-BN, and bilayer Gr-h-BN is about 3.2 Å, 3.3 Å, and 3.3 Å, respectively. The Gr (h-BN) sheet in the MTJs shows slight corrugations (about 0.1 ∼ 0.2 Å). As a result of the strong coupling between Ni (Co/Fe) and the bilayer sheet, the B, C, and N atoms show an induced magnetic moment, as shown in Table 1 and Table S1.

To investigate the stability of the two probe systems, the binding energy of the Co/Fe intercalated MTJs is:

$$E_b = E_{tot} - E_{TM} - E_{Gr} - E_{BN} - E_{electrode} \tag{2}$$

where E_{tot} represents total energy of the MTJs, E_{TM}, E_{Gr}, E_{BN}, and $E_{electrode}$ are the total energy of Co/Fe atom, graphene sheet, h-BN sheet, and Ni(111) electrode, respectively. The binding energy of the MTJs is shown in Table 1 and Table S1. Co/Fe intercalated MTJs are more stable (about 0.4 ∼ 0.7 eV) than the unintercalated MTJs. Such stability is produced by the strong coupling between intercalated Co/Fe and the bilayer systems. The Ni|BN-Co-Gr|Ni MTJs is the most stable Co intercalated configuration. Whereas the Ni|BN-Fe-BN|Ni MTJs is the most stable Fe intercalated configuration.

The magnetic properties of B, C, N, and Co/Fe atoms in the TM intercalated MTJs are shown in Table 1 and Table S1. The Co/Fe atom shows antiferromagnetic coupling with its nearest neighbor atoms resulting in small magnetic moments in the Co/Fe intercalated MTJs. For Ni|BN-Gr|Ni MTJs, the h-BN and Gr show very small corrugations, and the B atom is 0.11 Å closer to the Ni(111) surfaces than the N atom. The magnetic moments of the B and C atoms close to the Ni(111) for Ni|BN-Gr|Ni MTJs