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Full Length Article

Spin-polarized quantum transport in Fe_4N based current-perpendicular-to-plane spin valve

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ABSTRACT

Fe_4N has been confirmed to possess high spin polarization of 81.3% and low Gilbert damping constant of 0.021 ± 0.02 in the recent experiment. To explore the potential applications of Fe_4N in spintronics devices, the current-perpendicular-to-plane spin valve employing Fe_4N as electrode and Ag as spacer is simulated to study the spin polarized quantum transport by utilizing the first principles calculations combined with nonequilibrium Green's function. The project density of states (PDOS), transmission coefficient, spin-polarized current, magnetoresistance (MR) ratio and spin injection efficiency (SIE) as a function of bias voltage are studied. Our calculations reveal that spin down electron is the majority spin polarized electron and the absolute value of MR ratio of Fe_4N/Ag/Fe_4N at equilibrium reaches up to 174%, and it decreases with the bias increases. Besides, our results indicate that Fe_4N/Ag/Fe_4N device has stable SIE value of about 40% and stable MR ratios of about 150% when bias increases from 0 V to 0.1 V, and the device has a better performance within this voltage range.

1. Introduction

Spintronics, which utilize the spin degree of freedom, attracted much attention for decades [1–6]. Current-perpendicular-to-plane spin valves (CPP-SV) is regarded as one of the most significant spintronics device, the kernel construction of a CPP-SV consists of two magnetic layers separated by a nonmagnetic metallic layer. One magnetic layer has free magnetization direction to respond to magnetic flux from magnetic data bits, while the magnetization direction of the other magnetic layer is fixed by an antiferromagnetic layer. Owing to the lower sensor resistance, CPP-SV possesses lower electric noise, and it has great potential in application of an ultra-high-speed reading in magnetic read heads of hard disk drivers as well as spin transfer torque (STT) devices in spin random access memory [7–9]. The electronic and magnetic properties of heterostructures have been studied in detail [10–16]. While the injection and detection of highly polarized spin current is still one of the foremost challenges of CPP-SV. In addition, interface properties are very important in CPP-SV [17]. According to Valet-Fert model [18], the magnetoresistance (MR) ratio severely depends on interfacial spin asymmetry coefficients, and interface electronic structure could dominate electron tunneling. Employing ferromagnets with high spin polarization as electrode material is essential for a CPP-SV to achieve a high magnetoresistance (MR). Some ferromagnets such as Heusler alloys Co_2MnSi [19,20], $Co_2FeGe_{0.5}Ga_{0.5}$ [21] have been experimentally applied to CPP-SV device, and quaternary Heusler alloys such as CoFeMnSi [22–25] and MCoVZ (M = Lu, Y; Z = Si, Ge) [26] have received theoretical investigation and are considered to be promising electrode materials for spintronics devices. In addition, materials consisting of magnetic elements and light elements, such as ferromagnetic iron nitrides have been under intense investigation [27,28]. In particular, Fe_4N with a perovskite type structure where N is located at the body centre position of the fcc-Fe has advantages of simple crystalline, inexpensive, low coercivity, high Curie temperature of 761 K, and low synthesis temperature [29–33]. Electronic structure, magnetic properties and hyperfine interactions of Fe_4N are investigated [34,35] and it has been theoretically predicted to possess high polarization [31], and inverse anisotropic magnetoresistance attributing to negative interfacial spin scattering asymmetry has been observed in experiments [36–39]. Such inverse MR effect is useful for novel magnetic logic circuits [40].

More recently, a low Gilbert damping constant (α = 0.021 ± 0.02) of Fe_4N has been experimentally measured by ferromagnetic resonance [41]. Besides, the experiment indicated that Fe_4N film grown on Ag buffer layer has a better texture, and spin polarization of 81.3% is detected by using point contact Andreev reflection (PCAR) measurement, which is the highest experimental value for Fe_4N up to now [42]. It indicates that Fe_4N is one of the most promising candidates to be electrode materials [43–47], and it is crucial for understanding spin

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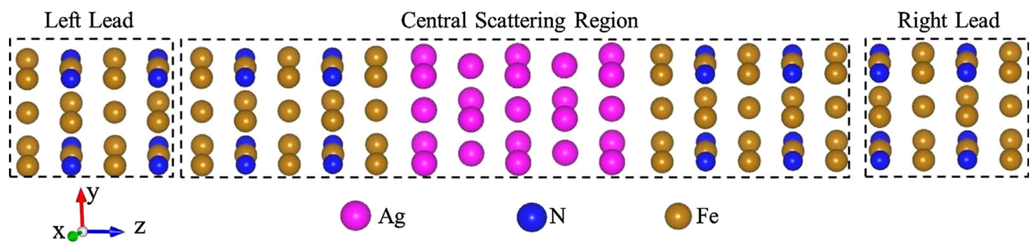

Fig. 1. Schematic illustration of the $Fe_4N/Ag/Fe_4N$ CPP-SV. The *z*-axis is the transport direction.

injection and magnetoresistance of a CPP-SV based on Fe_4N. In this paper, we perform first-principles calculations combined with nonequilibrium Green's function method to study the spin transport properties in CPP-SV $Fe_4N/Ag/Fe_4N$.

2. Computational method

In Fig. 1, two-probe current-perpendicular-to-plane spin valve (CPP-SV) device model consisting of two semi-infinite Fe_4N electrodes sandwiching 5 Ag layers is built, and the model is divided in to left electrode, central scattering region and right electrode. The in-plane lattice constant of the junction is fixed at 3.795 Å which is the experimental value of Fe_4N, thus the lattice mismatch between Fe_4N and Ag (4.079 Å) is about 7%. The interface relaxation is firstly performed by using VASP package based on density functional theory (DFT) [48,49]. The SCF convergence criterion of 10^{-6} eV and mesh of 9 × 9 × 1 Monkhorst-Pack k-points in Brillouin zone are applied, and the cutoff energy is set to 500 eV. The optimized distance between Fe and Ag atom is found to be 2.63 Å. The spin-dependent transport properties calculations are based on a state-of-the-art technique where DFT is combined with the Keldysh nonequilibrium Green's function (NEGF) theory, as implemented in Nanodcal package [50,51]. In our work, the CPP-SV is periodic along the *x*- and *y* axes, while the transport direction is along the *z* axis.

3. Results and discussion

Firstly, we discuss spin transportation at equilibrium. Fig. 2 exhibits the project density of states (PDOS) of $Fe_4N/Ag/Fe_4N$ junction at equilibrium by different colors on a logarithmic scale along the transport direction (*z* direction). (i) When magnetic moments of the two magnetic electrodes are in antiparallel configuration (APC), there are larger spin up states exist in the right electrode which could accommodate spin up electrons. However, the left electrode has smaller spin up states, indicating that it offers few spin up electrons. Besides, there are larger spin down states at left electrodes which means it could generate spin down electrons, while there are few states to accommodate these spin down electrons due to the reason that the right electrode has smaller spin down states. Therefore, such asymmetric PDOSs distribution suppresses the spin transport, and there are few spin polarized current could be detected, resulting in a high resistance state of the $Fe_4N/Ag/Fe_4N$ junction. (ii) When magnetic moment of the two magnetic electrodes is in parallel configuration (PC), spin up electrons possess few states at both left and right electrodes, indicating that they could hardly tunnel through the Ag spacer. Besides, spin down electrons from the left electrode enter Ag spacer with a larger DOSs, and then flow into the right electrode with a larger DOSs. It means spin down electrons traverse via the Fe_4N electrodes by tunnelling through the Ag spacer, and the junction switches into a low resistance state, and spin down electrons have majority DOSs to dominate transport.

In our two-probe device model, the transport coefficients have been calculated based on converged SCF calculations of two electrodes and centre scattering region. The spin-dependent transmission coefficient$T^{\sigma}(E)$ can be defined as

$$T^{\sigma}(E) = \frac{1}{N^2}\int d^2k_{//}T^{\sigma}(\overrightarrow{k_{//}}, E) \tag{1}$$

where $N^2 = N \times N$ represents the number of sampling point in the two-dimensional (2-D) Brillouin zone (BZ), and $\overrightarrow{k_{//}} = (k_x, k_y)$ is the in-plane electron wave vector which states a point in 2-D BZ, and σ indicates

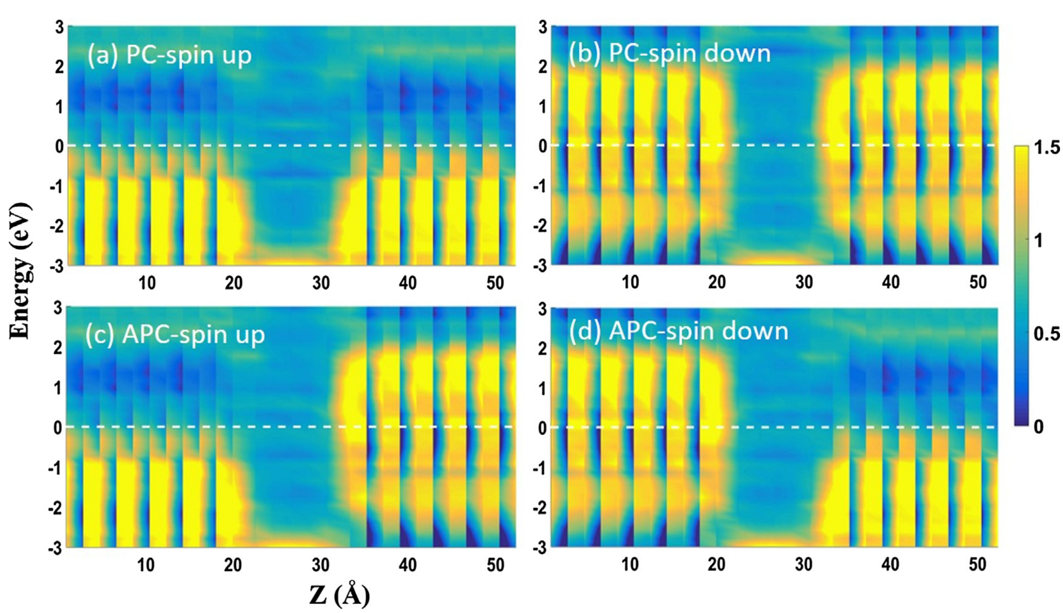

Fig. 2. Project density of states (PDOS) by different colors on a logarithmic scale along the transport direction (*z*-axis) of the $Fe_4N/Ag/Fe_4N$ CPP-SV at equilibrium.