Spin-transfer torques in anti-ferromagnetic metals from first principles

Yuan Xu, Shuai Wang, and Ke Xia
State Key Laboratory for Surface Physics, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China
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In spite of the absence of a macroscopic magnetic moment, an anti-ferromagnet is spin-polarized on an atomic scale. The electric current passing through a conducting anti-ferromagnet is polarized as well, leading to spin-transfer torques when the order parameter is textured, such as in anti-ferromagnetic non-collinear spin valves and domain walls. We report a first principles study on the electronic transport properties of anti-ferromagnetic systems. The current-induced spin torques acting on the magnetic moments are comparable with those in conventional ferromagnetic materials, leading to measurable angular resistances and current-induced magnetization dynamics. In contrast to ferromagnets, spin torques in anti-ferromagnets are very nonlocal. The torques acting far away from the center of an anti-ferromagnetic domain wall should facilitate current-induced domain wall motion.

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Anti-ferromagnet metals (AFMs) are widely used to pin and exchange-bias ferromagnets in devices such as magnetic spin valve read heads [1, 2]. The absence of magnetic stray fields makes them very useful as probes tips in spin-polarized scanning tunnelling microscopes [3]. AFMs are materials with spontaneous magnetization below a critical Néel temperature at which the magnetic moments of two (or more) sub-lattices point into opposite directions, such that the net magnetic moment of AFM vanishes. External magnetic fields cannot be used to manipulate the strongly coupled magnetic moments of AFMs. An alternative for magnetic fields to excite ferromagnets (FMs) is the current-induced spin-transfer torque (STT) [4]. Since the electric current is spin-polarized on an atomic scale, the STT phenomenon may excite the anti-ferromagnetic order parameter. It is not obvious whether the STT is strong enough and how different sub-lattices are affected.

Recent theoretical studies [5, 6, 7] predicted that in spin valves with uncompensated anti-ferromagnets angular resistance (AR) effect can be expected. Reversal of the anti-ferromagnetic order parameter is equivalent with a phase shift by a half period. Furthermore, STT is not an interface effect as in ferromagnets, but effective over the whole AFM. Very recently, strong experimental evidences of STT between AFM and FM have been reported [8]. In addition, the resistance of anti-ferromagnetic domain walls (AFDWs) in chromium has been measured [9]. In contrast to FMs, AFMs have much smaller shape anisotropies which makes manipulation of its magnetic moments easier — provided one can apply a sizable spin torque on the moments. What is the magnitude of the spin torque for an atomic scale spin polarization? Can an atomic scale spin polarization gives rise to observable AR effect? These are the questions we attempt to answer in this work.

γ-FeMn is an AFM used as pinning layer in spin valves, and we demonstrate that an electric current can induce angular momentum transfer between magnetic moments in AFMs. By a detailed analysis of the current and non-equilibrium charge densities, we show that an atomic scale spin polarization exists even for compensated AFMs. A sizable AR is predicted in anti-ferromagnetic spin valves (AFSVs). In an AFDW the spin torque is effective not only around the domain wall center but throughout the entire AFM, which can be understood by the suppressed spin precession.

In our calculations, the atomic potential was determined in the framework of the tight-binding (TB) linear muffin-tin-orbital (MTO) method based on density functional theory in the local density approximation [10] and an exchange-correlation potential parameterized by von Barth and Hedin [11]. The self-consistent crystal potentials were used as input to a TB-MTO wave-function-matching calculation and the scattering wave functions of the whole system were obtained explicitly [12]. To model non-collinear magnetic configurations in AFDWs, a rigid potential approximation is applied, which is a good approximation for sufficiently wide domain walls [13].

![FIG. 1](color online) (a) Magnetic structure of γ-FeMn. (b) fcc(111) plane of γ-FeMn, where the dashed lines connect the atoms in a unit cell.

The spin current and charge density can be calculated from the scattering wave functions. The torques acting on an atomic plane are defined as the difference between incoming and outgoing spin current [14]. Finally, we focus on transport along the direction perpendicular to the plane fcc(111) as illustrated in Fig.1(b), where...
between both order parameters. In our calculations, the FeMn serves as the fixed layer and FeMn2 as the free layer. The magnetic moments of Fe1 and Mn2 point into opposite directions. Our calculation yields the magnetic moments as \( m_{Fe} = 1.4 \mu_B \) and \( m_{Mn} = 1.9 \mu_B \).

When a current passes through an anti-ferromagnetic material, the current-induced non-equilibrium charge density integrated over the atomic sphere of an atom is spin-polarized. We define the polarization of atom \( \alpha \) as \( P_{\alpha} = (\rho_{\uparrow\alpha} - \rho_{\downarrow\alpha})/(\rho_{\uparrow\alpha} + \rho_{\downarrow\alpha}) \), where \( \rho_{\uparrow\alpha} \) is the spin resolved non-equilibrium charge density. \( \downarrow(\uparrow) \) indicates the electron spin parallel or antiparallel to the spin quantization axis.

In Fig.2 we plot \( P_{\alpha} \) for a single FeMn/Cu interface. We group the system into four inequivalent sub-lattices according to the inequivalent atoms in the unit cell of \( \gamma \)-FeMn. A nonzero polarization is found even at the Cu side. The sum of the spin polarizations of the four sub-lattices vanishes in each layer. These results show that a compensated anti-ferromagnet injects a spin polarization into a normal metal that oscillates on an atomic scale.

Let us consider now an AFSV denoted as FeMn1(\( \theta \)|Cu)|FeMn2|Cu, where an infinitely thick FeMn1 serves as the fixed layer and FeMn2 as the free layer. The \( z \) axis of spin space is set along the magnetization of the free layer and \( \theta \) gives the relative angle between both order parameters. In our calculations, the thicknesses of the Cu spacer and the FeMn2 free layer are chosen to be both 10 monolayers (ML).

The top panel of Fig.3 illustrates the magnetic structure of the so-called parallel configuration (\( \theta = 0^\circ \)). Here and in the following we group the four sub-lattices into two according to the direction of their magnetic moments. When the magnetization of FeMn1 is rotated from \( \theta = 0^\circ \) to \( \theta = 180^\circ \) (the antiparallel configuration), the electric resistance changes.

The bottom panel of Fig.3 gives the spin-polarized current at the two sub-lattices. When the magnetizations of the two AFM layers are collinear, there is no net current spin polarization. However, the spatial distribution of spin-polarized current is not trivial. In fact, the spin-polarized currents on the two sub-lattices do not vanish even in Cu. They are identical in magnitude but oppositely spin-polarized. Another finding is that the spin-polarized current oscillates between the two sub-lattices and is not conserved within one sub-lattice.

The AR ratio in terms of conductance as \( |G(0^\circ) - G(180^\circ)|/G(180^\circ) \) amounts to a measurable 5%. The remaining question is the robustness of this AR effect in the presence of interfacial disorder. We modelled disorder by an interfacial alloy with a lateral super-cell method. For a 1ML (FeMn)\( _{1-x} \)Cu \( _x \) interfacial alloy, the AR dependence on interfacial alloy concentration \( x \) is shown in Fig.4, which indicates that the AR is somewhat suppressed in the presence of disorder, but should remain to be observable.

It is interesting to investigate the STT due to the atomic scale spin dependent scattering. Before going into the numerical results, we analyze the symmetry of the STT. For one sub-lattice, similar to that of FM, the
torque on a local magnetic moment $\mathbf{m}$ is proportional to $\mathbf{m} \times \mathbf{M} \times \mathbf{m}$ (in-plane) and $\mathbf{m} \times \mathbf{M}$ (out-of-plane), where $\mathbf{M}$ denotes the source of spin current. For another sub-lattice, both $\mathbf{m}$ and $\mathbf{M}$ are reversed. The in-plane torque is also reversed whereas the out-of-plane torque remains unchanged. Because the in-plane torque $T_{\parallel}$ on two sub-lattices are identical in magnitude and opposite in direction and the magnetization of two sub-lattices points into opposite directions, the net effect of STT tends to rotate those moments together. In contrast to $T_{\parallel}$, the out-of-plane torque $T_{\perp}$ acts identically on the two magnetic sub-lattices. As the exchange coupling in the AFM is strong, out-of-plane torques will not result in any significant effect on the dynamics of the magnetic moments.

As shown in Fig 5(a), the spin torque in the AFM layer oscillates deep into material which differs from conventional FM spin valve. The angular dependence of the total in-plane torque acting on sub-lattice (Fe1&Mn2) in FeMn2 is shown in Fig 5(b). For $\theta = 150^\circ$, the torque ($4.1 \times 10^{-3}eV_{f/\mu_B}$) acting on the surface atoms is much smaller than that in FM spin valve ($\sim 10^{-3}eV_{f/\mu_B}$). However, due to slow decay of the spin torque in AFMs, the integrated torque on per atom of AFMs ($2.4 \times 10^{-4}eV_{f/\mu_B}$) is comparable to that in FMs.

Similar spin transfer effect should occur in AFDWs. As domain wall physics in AFMs has not been fully understood, we simply consider a Bloch-like domain wall which could exist in the experiment. The configuration is described by $\theta(y) = \frac{\pi}{2} + \arcsin[\tanh(\frac{y-y_0}{\lambda_{DW}})]$, where $\lambda_{DW}$ is the characteristic length which is selected to be 4ML and $y_0$ the center of the wall. The spin direction in each monolayer along the wall is shown in Fig 5(b). The change of the total conductance due to the formation of a wall is 2.8% for a 4ML thick domain wall, which is comparable to that in a FM with the same width.

Fig 6(c) shows the in-plane torque exerted on one sub-lattice (Fe1&Mn2) as a function of position in the domain wall. There is a substantial STT in the region far away from the domain wall center. This is attributed to the spin degeneracy of the electronic band structure in the AFM. The injected spin can penetrate and precess coherently until deep into the AFM. As a result, STT in AFM is very non-local, at least in the absence of disorder scattering.

We investigate the dynamics of the AFDW with the Landau-Lifshitz-Gilbert (LLG) equation using our calculated STT. An AFM with two sub-lattices is described by two sets of coupled LLG equations. Here we decouple the equations by assuming that the magnetizations of two sub-lattices in the same layer are antiparallel to each other at any time. This should be reasonable due to a strong anti-ferromagnetic coupling between the two sub-lattices.

To investigate dynamics of the domain wall in the presence of a current, we follow the method of Ohe and Kramer who studied FM domain walls. This method consists of several steps: (i) Given a domain wall configuration, we calculate the STT acting on each site under a certain current density; (ii) the obtained spin torque at each site is substituted into the LLG equation to obtain a set of equations for each site in the domain wall at a given time $t$; (iii) by integrating the LLG equation, we
We first obtain the domain wall configuration after an interval at $t' = t + \delta t$; (iv) once a new domain wall configuration is obtained, we can calculate the STT again and the process is repeated. The interval $\delta t$ between two consecutive steps is chosen small enough to guarantee numerical convergence of the solution.

In particular, a magnetic anisotropy constant of $1.35 \times 10^5 \text{ erg/cm}^3$, exchange stiffness constant of $0.94 \times 10^{-9} \text{ erg/cm}$, magnetization of sub-lattice of 650 Gs and Gilbert damping constant of 0.1 are used in our calculation.

Under a current density of $5 \times 10^7 \text{ A/cm}^2$ and starting from the initial domain wall configuration mentioned above, we obtained results for 10 time steps of $\delta t = 2$ ps. The domain wall moves into the $-Y$ direction and the estimated velocity is 4 m/s. In contrast to the FM domain wall, the velocity is maintained due to the vanishing de-magnetization field. For the same reason, when no pinning field is taken into account, the critical current that sets the AFDW into motion is also expected to be very small as compared to a FM domain wall.

In summary, we find an atomic scale spin polarization in completely compensated AFMs. An STT can be induced by an electric bias. In AFSVs, a sizable AR is predicted and the STT is found to be comparable to that in conventional FM spin valves. In AFDWs, the torques turn out to be nonlocal. The spin dynamics of AFDWs is studied by including the STT into the LLG equation for AFMs.

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