Intrinsic life-time and external manipulation of Néel states in antiferromagnetic adatom spins on semiconductor surfaces

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Abstract
It has been proposed that antiferromagnetic Fe adatom spins on semiconductor Cu–N surfaces can be used to store information (Loth et al 2012 Science 335 196). Here, we investigate spin dynamics of such antiferromagnetic systems through Monte Carlo simulations. We find out the temperature and size laws of switching rates of Néel states and show that the Néel states can become stable enough for the information storage when the number of spins reaches one or two dozens of the Fe spins. We also explore promising methods for manipulating the Néel states. These could help realize information storage with such antiferromagnetic spin systems.

Keywords: nanomagnetism, neel state, semiconductor surface

1. Introduction
The atomic-size antiferromagnets (AFM) on semiconductor surfaces have been realized thanks to technology advancement, and have attracted a lot of attention for their potential in magnetic storage technology [1–5]. Due to insensitivity to magnetic fields, these nanomagnets are considered to be able to meet the needs of the vast growth of storage density in magnetic media [6]. On the other hand, it is also far more difficult to effectively manipulate the AFM stagger magnetization (or Néel state) than ferromagnetic magnetization in ferromagnetic materials. Modern scanning tunneling microscopy (STM) technology can be used to manipulate magnetic states of such nanomagnets through applying an electric field or injecting an electron current on one of the adatom spins [5–9]. It has been reported that AFM chains assembled by placing Fe adatoms on a Cu$_2$N overlayer on Cu(1 0 0) can be switched between two quasistable Néel states when the polarized electrons are made to flow across one atom of the chain [7]. There have been theoretical studies on magnetic transitions induced by tunneling electrons [10–14], but temperature effects need to be considered. A reliable study on the temperature-dependent dynamics of Néel states is needed.

Here, we use the dynamic Monte Carlo method to study the switching rates of a series of such antiferromagnetic Fe spin chains. We investigate effects of various temperatures and spin-polarized currents in terms of experimental parameters. Arrhenius-like behaviors are observed until the temperature is too low to hurdle the thermal activation barrier of the spin reversal. Our results show that such spin chains can be stable enough for practical usage when one or two dozen Fe adatoms are used. We also explore effective methods for external manipulation of the Néel states. More detailed results will be presented in the following.

2. Spin model and simulation method
For low temperatures ($T < 10$ K), the Fe spin bi-chains on the CuN/Cu(100) surface can be effectively described with an anisotropic Heisenberg antiferromagnetic model of $S = 2$ [7, 8],

$$\hat{H}_0 = \sum_{i,j} \left( \hat{J}_i \hat{S}_i \cdot \hat{S}_{i+1,j} \right) - \sum_i \hat{J}_i \hat{S}_i \cdot \hat{S}_{2}$$

(1)

where
of the Néel states (more detail will be given in the following), and they are updated at each step of the Monte Carlo simulation. For each electron tunneling from the STM tip through the first Fe atom and into the substrate, there is a chance to change the states of the whole Fe spin chains.

For our DMC simulation, the MC steps are defined by the time points: \( t_n = \Delta t \cdot n \), where \( n \) takes non-negative integers in sequence. The \( \Delta t \) is set to \( 1.6 \times 10^{-7} \) s or determined by \( \Delta t = 1/eI \), where \( I \) is the current intensity from the STM tips. \( \Delta t \) is chosen to satisfy the requirement that there is only one electron within a MC step. At the beginning, we set all of the spins at one for Néel state \( \hat{E}_0 \) and the Nth spin should be set as \((-1)^N \cdot S\). For the nth step, the MC simulations are performed in the following way.

For each Fe spin, we take \( \hat{H}_{ij} \) as a 5 states quantum model, and there is a thermal-activated energy barrier \( \Delta \varepsilon \) between the starting and ending states. Using the Arrhenius law [15, 16], we obtain the thermal-activated spin reversal probability, \( P_1 = 1 - \exp(-\Delta \varepsilon) \), for each MC step [17–19], where \( r = r_0 \exp(-\Delta \varepsilon/k_{B}T) \) is the spin reversal rate and \( r_0 \) is the character attempt frequency. When an injected electron is tunneling through the first Fe spin, the collision channel states \( S_0 \) are defined to simulate the electron–Fe–spin coupling, and the electron-activated spin reversal probability is defined as \( P_2 \) [14, 20, 23]. Therefore, the total probability for the first Fe spin is equivalent to \( P_1 = 1 - (1 - P_1)(1 - P_2) \). Actually, at extra-low temperature an additional collective spin channel becomes available for the system to transit from one Néel state to the other. This transition probability, calculated through exact diagonalization of the Hamiltonian, is added to the above probability to completely describe the spin dynamics.

For the nth MC step, each spin in the system has a chance to reverse. With \( n \) increasing, at last, the system finally transits to the other Néel state \( \hat{E}_1 \) at a special \( n \). This \( n \) value is denoted by \( N_i \). We define \( \eta_i = (N_i) \cdot \Delta t \) as the average transition time from \( \hat{E}_0 \) to \( \hat{E}_1 \). The average transition time from \( \hat{E}_1 \) to \( \hat{E}_0 \) is calculated in the same way. The switching rate is defined as \( R = 2(\eta_1 + \eta_2) \). To be consistent with experiment [7, 8], we take \( J = 0.737 \) meV, \( J' = 0.03 \) meV, \( D = 1.87 \) meV, \( E = 0.061 \) meV, \( B_{zp} = 0.115 \) tesla, and \( r_0 = 2 \times 10^8 \) s\(^{-1} \) in the following. Our main results are calculated by averaging over 100 000 runs of DMC simulations.

3. Intrinsic lifetimes of Néel states

We simulate the spin dynamics for the different Fe chains with magnetic fields. It is confirmed that the magnetic field has little effect on switching rates. Simulated switching rates for \( 1 \times N \) Fe-spin chains are presented in figure 2(a). It is clear that the switching rates show strong temperature dependence as expected. Above 6 K, the switching rates of the \( 1 \times N \) Fe chains mainly follow the Arrhenius law. With the addition of two Fe spins, the energy barrier increases with 4.15 meV. The switching rates of Néel states in long Fe chains are tiny in comparison with those in short ones. When temperature decreases away from the Arrhenius regime, the switching rates become
chains are shown in figure 2(b). In these cases, the low temperature limit of the 10 linear chains, with 1 chain to be bi-chains with d. Although increasing temperature will decrease the temperature-rate curves of single chains for below about 2 K. It should be pointed out that the simulated lifetime of the Néel states can be considered to be quite stable small that the Néel state, we define a Néel weight which is in good agreement with the experimental value [7]. With all the three parameters known, we can calculate lifetimes (τ = 1/R) of Néel states for any given temperature and chain length. For the ultra-low temperature limit (0 K), we have 0.12 s, 1.8 min, 1.0 d, and 2.1 years for the 1 × N chains with N = 6, 8, 10, and 12, respectively. For the 2 × N chains, we have R0 = 2.0 × 10^-8 per second, and the Néel dependence relations of ΔE and τ0 (R0) are similar to equation (4). For a special case of 2 × N (N = 8) chains, we already have τ0 ≈ 28.2 d. Although increasing temperature will decrease the lifetime, a very long life time of a few years can be achieved as long as N is large enough, making 1 × 14 and 2 × 8 or longer chains.

4. Manipulation of Néel states

A current injected through the STM tip on the first adatom spin can change the Néel states in the Fe spin chains [7, 14]. To characterize a Néel state, we define a Néel weight W0 of the 1 × N chain to be \( \sum (-1)^i S_i / S \) with i running from 1 to N. It is N and ~N for the Néel states \( E_0 \) and \( E_1 \), respectively. We present the Néel weight W0 of 1 × 8 spin chain under different current intensities and temperatures in figure 4(a). It can be seen that the Néel weight changes exponentially with time. The temperature and the spin-polarized current play the key role in determining the switching rates and target Néel

\[
\Delta E = 2.07 \cdot N - 4.37, \quad \tau_0 = 2.97 \times 10^{-10} \times 27.9^N.
\]

Figure 2. Temperature dependence of the switching rates without magnetic field for 1 × N linear chains with N = 4, 6, 8, and 10 (a); and 2 × N bi-chains with N = 4, 6, 8, and 10 (b).

Figure 3. The energy barrier (ΔE) and the residual switching rates (Rt) (a), and the lifetimes (τ) (b) of the 1 × N Fe linear chains, with N taking even numbers.
weights, but the initial status of Néel weights, \( \eta_0 \), do not affect the target Néel weights (\( W_{\infty} \)). Generally, we can fit the time-dependent Néel weights with a simple function:

\[
W_T = W_0 \exp(-t/\tau_0) + W_{\infty}.
\]  

(5)

The \( \tau_0 \) parameter describes the timescale, and \( W_0 + W_{\infty} \) is equivalent to the initial Néel weight. The calculated three fitting parameters are compared in Table 1 between different temperatures, different currents, and different initial Néel weights. The temperature dependence of the target Néel weights for four currents (1, 2, 4, and 8 pA) is presented in Figure 4(b). The current dependence of the target Néel weights for different temperatures (6, 8, and 10 K) is presented in Figure 4(c). It is clear that the temperature dependence is weak, but the target Néel weight increases substantially when the current intensity increases. It is interesting that there exists a big \( W_{\infty} \) step at ~6 pA. It is because one more spin channel becomes available at the equivalent voltage for inelastic tunneling of the electrons [24, 25].

The sensitive current dependence of the target Néel weights can be used to manipulate the Néel states through suitable spin-polarized currents and temperatures. When a periodic spin-polarized current between -8 and 8 pA is applied, the Néel weights can assume a cyclic periodic function. Such manipulation of the \( 1 \times N \) chains (\( N = 4, 8 \)) with two currents with different time periods is presented in Figures 5(a) and (b). The Néel states are almost fully switched for these two cases. The two curves look similar although the timescales are hugely different from each other. Furthermore, the big step in the \( I - W_{\infty} \) curves in Figure 4(c) can be used to manipulate the Néel states. When the current is periodically switched between 6.2 pA and 5.8 pA, the Néel weight is periodically switched between 5.1 and 7.9, as shown in Figure 5(c).

5. Discussion and conclusion

It was pointed out by Gauyacq et al [14] that there are three mechanisms for electron-induced switching between the Néel states of Fe antiferromagnetic chains. At finite temperature, thermal effects will go into action and increase...
exponentially with temperature. They can be attributed to a barrier-hurdling thermal activation mechanism described by an Arrhenius law.

In summary, we have investigated spin dynamics of the antiferromagnetic spin systems through Monte Carlo simulations. We have found out the temperature and size laws of switching rates of Néel states for such spin systems. Furthermore, we have shown that the Néel states can be made stable enough for the information storage if one or two dozens of such Fe spins are used. We also have demonstrated promising methods for manipulating the Néel states. We believe that these can be useful to realize antiferromagnetic information storage.

Acknowledgments

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