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Tip-surface interaction and rate of magnetic transitions

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Abstract. Calculations of the interaction between a magnetic tip of an atomic force microscope with a magnetic surface using the non-collinear extension of the Alexander-Anderson model are described. The mechanism and rate of thermally activated magnetic transitions in a cluster of atoms at the tip is investigated. The results are compared with experimental data and found to be in good agreement with measured lifetimes [R. Schmidt *et. al.*, *Phys. Rev. B* 86, 174402 (2012).]. The results are also compared with previously reported density functional theory calculations.

1. Introduction

Magnetic exchange force microscopy (MExFM) makes it possible to detect the magnetic exchange force between a magnetic tip and a magnetic surface with atomic resolution [1-3]. In a recent experiment [2, 3], a ferromagnetic tip was scanned over an antiferromagnetic Fe layer on a W(001) substrate. The image of the surface shows an alternating pattern since the tip-surface exchange interaction is favorable for surface atoms with one direction of the magnetic moment and unfavorable for the other surface atoms. The strength of the interaction depends on the distance between the tip and the surface. Later, it was shown that the magnetic state of the small cluster supported at the tip can switch with time and that its average lifetime depends strongly on the tip-surface distance [4]. This illustrates the effect of the exchange interaction on the lifetime of the magnetic state and suggests a possible way to record and read data.

Theoretical calculations based on density functional theory (DFT) have been carried out to help interpret the results of such experiments [2,3,5]. The tip was modeled as a square pyramidal arrangement of 14 Fe, Cr or Mn atoms. The results of the calculations showed that an antiferromagnetic alignment of the tip and the underlying surface atom is of lower energy than ferromagnetic alignment. This was also found to be the case when the tip was represented by a single Fe, Cr or Mn atom. The calculations did not address the mechanism and rate of the magnetic transitions.

2. Methodology

The simulations presented here made use of the non-collinear extension of the Alexander-Anderson (NCAA) model [6,7]. Two types of simulations of the system were carried out. In one case, the total number of d-electrons in the system was fixed. In the other case, the d-electron energy level was fixed with respect to the Fermi level and the number of d-electrons found from self-consistency calculations for each atom. Electroneutrality is ensured in that case by transfer of s(p) electrons to or from the bath of the extended metal. The effect of the exchange interaction and thereby the distance between the tip and the surface on the thermally activated transitions in the magnetic cluster at the tip is calculated.

The magnetic cluster at the tip was represented either by a single Fe, Mn or Cr atom or by a square pyramidal arrangement of 14 Fe atoms. The surface was represented by a layer of 13 Fe atoms when the tip consisted of a single atom, but by a layer of 25 atoms when the larger, 14 atom tip was simulated. The underlying substrate is effectively taken into account in the NCAA model through a hybridization parameter and the Fermi level. The larger tip cluster model was used in calculations of the lifetime of the magnetic states.

The rate of magnetic transitions in the tip was calculated by first finding the minimum energy path (MEP) between the ferromagnetic and antiferromagnetic states of the tip cluster with respect to the underlying surface atom. The geodesic nudged elastic band method [8] was used to find the MEPs. The maximum energy along the MEP corresponds to a first order saddle point on the energy surface and gives an estimate of the activation energy. The pre-exponential factor was calculated using harmonic transition state theory (HTST) for magnetic systems [9] which gives an Arrhenius expression for the transition rate. The corresponding expression for the average lifetime, τ, of a magnetic state is:

$$\tau = \tau_0 \exp\left(\frac{E_a}{k_B T}\right),$$

where E_a the activation energy, k_B the Boltzmann constant and T the temperature. The pre-exponential factor τ_0 is calculated from the curvature of the energy surface at the saddle point and at the initial state minimum [9].

3. Results

3.1. Tip-surface interaction

The tip-surface exchange energy is the energy difference between a parallel and antiparallel alignment of the magnetic vectors at the tip with respect to the magnetic vector of the underlying surface atom. When the exchange energy is positive, the ferromagnetic alignment is of lower energy than the antiferromagnetic one. Figure 1 shows the calculated exchange energy for a single atom representation of the tip as a function of the hopping parameter, *V*, in the NCAA model that represents the overlap of wave function of the tip atom with the wave function of the underlying surface atom. The closer the tip is to the surface the larger this overlap is and larger the hopping parameter. Results for Fe, Mn and Cr tip atom are shown. When the total number of d-electrons in the system is fixed, see figure 1(a), the exchange coupling is antiferromagnetic and the exchange interaction is weakest for Fe and strongest for Cr. This is similar to the results of the DFT calculations [5]. In this case, the maximum of absolute value of the exchange energy for the Cr tip is a factor of 20 larger than for Fe atom at the tip and a factor of 4 larger than for the Mn atom. However, when the Fermi level is fixed, see figure 1(b), and the number of d-electrons is found from self-consistency calculations for each value of the hopping parameter, the exchange energy is of opposite sign for a tip with an Fe and Mn atom, i.e. the interaction is ferromagnetic, and the exchange interaction for Fe is stronger than for Cr.

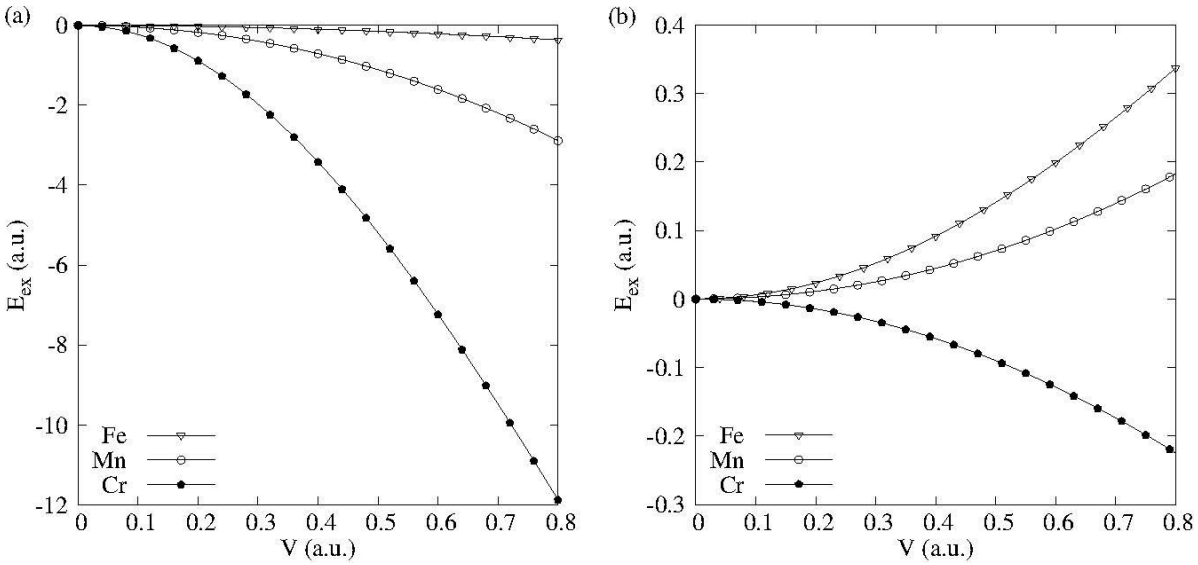

Figure 1. Exchange interaction between a magnetic tip and an underlying surface atom. The tip is represented by a single atom in this case, either an Fe, Mn, or Cr atom. The exchange energy is shown as a function of the hopping parameter, *V*, in the non-collinear Alexander Anderson model. A larger hopping parameter corresponds to shorter distance between the tip and the surface. (a) Calculated result for a fixed total number of d-electrons in the system. (b) Calculated results for a fixed Fermi level. The sign of the exchange interaction is different in the two cases for Fe and Mn tip.

The two different cases show a significant difference in the calculated exchange energy. When the total number of d-electrons in the system is fixed, the results are similar to the DFT results [2,3,5]. However, when the Fermi level is fixed, a different sign of the exchange interaction is obtained for the Fe and Mn tips. Similar reversal of the sign of the exchange interaction was found for larger models of the Fe and Mn tips. Fixing the Fermi level is a better representation of the experimental situation since the tip and substrate are macroscopic and contain a large number of itinerant s(p)-electrons. From the experiments it is not possible to tell whether the interaction is ferromagnetic or antiferromagnetic.

2.2. Thermally activated transitions

In these calculations the tip was modeled as a square pyramid of 14 Fe atoms and the Fermi level was fixed. The two magnetic states of the tip correspond to either parallel (P) or antiparallel (A) alignment with the magnetic vector of the underlying surface atom. If the tip does not interact with the surface, then the energy of these two states is the same. The MEP (figure 2, (1) solid line) has a maximum rise in energy of 23.3 meV. When the tip interacts with the surface, the energy of the P state becomes lower than that of the A state. The MEP is therefore no longer symmetric as shown in figure 2 ((2) dot-dashed line). The activation energy for the transition from the P state to the A state is 27.0 meV but 19.5 meV for the reverse transition. When an applied magnetic field in the direction of the tip is included, the energy of the two states is changed, as shown by the (3) dashed and (4) dotted lines in figure 2. If the magnetic field points in the direction of the P state, then the energy of this state is lowered while the energy of the A state is increased. The activation energy for the transition from P state to A state then increases but the activation energy for the back transition decreases. For a field of 1 T, the two energy barriers become 29.5 meV and 17.6 meV, respectively. If the magnetic field

points in the opposite direction of the P state, then the change in the energy barrier is opposite, namely the energy barrier for the transition from P state to A state decreases and the energy barrier for the back transition increases. They become 24.5 meV and 21.7 meV, respectively.

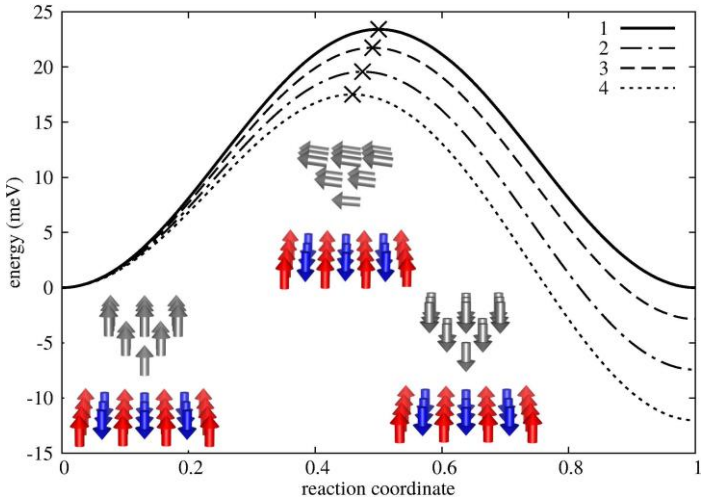

Figure 2. The minimum energy path for a transition between the magnetic states corresponding to antiparallel and parallel alignment of the 14 atoms tip with the underlying surface atom. The (1) full line corresponds to a tip that does not interact with a surface. The (2) dash-dotted line corresponds to a tip-surface separation of 450 pm. The (3) dashed and (4) dotted lines represent the system in a magnetic field of 1 T, pointing antiparallel and parallel to the tip, respectively. The maxima along the minimum energy paths are indicated with an x. They correspond to saddle points on the energy surface and give an estimate of the activation energy for the transition. The alignment of the magnetic vectors in the initial state, at the saddle points and in the final state is shown in the insets.

The pre-exponential factor was calculated and found to be $6 \cdot 10^{-11}$s for the isolated tip. The interaction with the surface changes this value insignificantly. Thus, at a temperature of 8.1 K, as in the experimental study, the lifetime of the magnetic state of the isolated tip is about 5 hours. When the tip is brought to a distance of about 450 pm from the surface, the average lifetime of the A state becomes 62 seconds and the lifetime of P state increases to 8 weeks. This means that a transition from the P state to A state will not occur on the time scale of the experiment, only transitions from A state to P state are fast enough. When a magnetic field of 1 T is included, the lifetimes of the metastable A state increases to 24 minutes and or decreases to 4 seconds depending on the direction of magnetic field. These results are consistent with the experimental observations of Schmidt *et. al.* [4]. They found the metastable tip state to have a lifetime of 27 ± 5 s and 17 ± 3 s. When the distance between tip and surface is taken to be 430 pm, the 14 atoms tip reproduces these times when a small magnetic field (60 mT) is included. The energy barrier for the A to P transition is then 18.9 meV and 18.6 meV, depending on the direction of the field.

4. Conclusion

The calculations described here largely support the interpretation of the experimental results of Schmidt *et. al.* [4]. Their assignment of the metastable and stable state in terms of the direction of the magnetic vectors of the tip, which was based on the results of the DFT calculations, is however different from our results because the sign of the exchange interaction is different when the Fermi

level is fixed as compared with a fixed total number of d-electrons. In the NCAA model it is assumed that the magnetic atoms interact with free s(p)-electrons of a non-magnetic metal and the energy of the localized electrons with respect to the Fermi level is a parameter. The two approaches, fixing the Fermi level and fixing the number of d-electrons, give different sign of the exchange energy for Fe and Mn tips. Since the DFT calculations [2,3,5] were carried out for a small system with an unsupported tip, they are closer to the NCAA simulations with a fixed number of d-electrons rather than the NCAA calculations with fixed Fermi level.

In order to estimate the thermal stability of the magnetic state of the tip, the geodesic nudged elastic band method was employed to calculate minimum energy paths for the transition. This gave estimates of the activation energy for various situations. The pre-exponential factor was calculated using harmonic transition state theory. A model of the ferromagnetic Fe tip consisting of 14 atoms and a tip-surface distance of 430 – 450 pm gave a lifetime of the metastable, A state in close agreement with the experimental observations [4]. The energy barrier was 23.3 meV for an isolated tip but decreased as the tip is brought close to the surface. By changing the tip-surface distance, the lifetime of the metastable state can be varied from seconds to hours.

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