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Theoretical study of exchange force between magnetic films

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We calculated the exchange force between two magnetic Fe films by first-principles calculations. It is shown that the exchange force is sensitive to the film-film separation and relative atomic site on the surface for d/t < 1, where d is the distance between surfaces of the two films and t the lattice constant of bulk Fe. Based on their results, the feasibility of exchange force microscopy (EFM), which probes the exchange force between the tip and the sample, was discussed.

Key words: exchange force, atomic force microscopy, exchange force microscopy, surface magnetic structure, first-principles calculation.

1. Introduction

The magnetic force microscopy (MFM) detects the force arising from the interaction between magnetic dipoles of a tip and a sample. However, determination of atomic spin structures by this technique is difficult since the magnetic dipole interaction is a long-range one. The typical tip-sample separations in the MFM are on the order of more than 10 nm and the spatial resolution is on the order of 10 to 100 nm. An improvement of the resolution might be made by probing the short-range exchange force.1,4

This paper describes a theoretical study on the exchange force between two magnetic Fe(001) films using first-principles calculations, to show the feasibility of the exchange force microscopy (EFM), which probes the exchange force between the tip and the sample.

2. Calculation Method

As a model of the tip and sample, we adopted two three-atomic-layer Fe(001) films, which are separated by distance d, as shown in Fig.1(a). Surface atoms of one film are assumed to be facing two high-symmetry surface sites, hollow site (H in Fig.1) and top site (T in Fig.1) on the surface of the other film. The transitional symmetry is preserved in the surface-normal (x) direction, in which a set of the two three-layer films is periodically located with a five-atomic-layer vacuum gap (repeated slab model). For a calculation of the electronic structure of the adopted films, we employ the local-spin-density approximation to the density-functional theory, and the FLAPW method with Hedin-Lundquist exchange correlation.6 Because bulk Fe is in the ferromagnetic ground state, magnetic moments in each three-layer film are taken to be in ferromagnetic alignment. As is concerned, we consider the parallel (P) and anti-parallel (AP) magnetic configurations, in order to calculate the exchange force between the two films. Our calculations are carried out by changing the film-film separation d from 1.4 to 5.0 Å with the assumption that the internal atomic coordinates in each film are rigidly fixed.

Fig.1. Schematic representation of two three-atom-layer Fe (001) films adopted for our calculation. (a) is a side view of the two films and (b) is a top view of the lower film, where H and T are the hollow site and the top site on the surface, respectively.

3. Results and Discussion

We discuss first a change of the electronic charge densities with respect to the film-films separation. Figure 2 shows the calculated charge-density distribution in the (110) plane for the magnetic configuration P, where a is the lattice constant of a bulk Fe (a=2.83 Å). The separation of d/a=0.5 corresponds to an interlayer distance of the bulk Fe. The proximity of the two films with the relative separation d/a<1 causes a charge accumulation between surface atoms of the two films. For these values of the separations, significant modification of the density distribution as well as corresponding changes of magnetic moments on the surface are observed.
Fig. 2. Charge densities of the two films in a (110) plane for the magnetic configuration P for (a) the hollow site and (b) the top site. Adjacent contour differs by a factor of 2^{1/2} (in unit of 10^{-3} electrons/a.u.).

On the other hand, no significant change of the d-electron state was observed for Δx<1.

The forces, \( F_F \) and \( F_{AP} \), acting on the film for the magnetic configurations P and AP are shown in Fig. 3 for (a) the hollow site and (b) the top site. The force direction is perpendicular to the film surface due to the symmetry. For each site, the forces \( F_F \) and \( F_{AP} \) have negative values, suggesting that attractive forces are dominant. The exchange force \( F_{ex} \), defined by \( F_{ex} = F_{AP} - F_F \), is also plotted in Fig. 3. The exchange force for Δx<1 arises from the direct exchange coupling between two films, making interactions very sensitive to the film-film separation and the surface site, as seen in Fig. 3. The magnitude of the exchange force variation relative to the surface site is on the order of \( 10^{-9} \) to \( 10^{-13} \) N. Since the force sensitivity of the conventional AFM is on the order of \( 10^{-12} \) to \( 10^{-15} \) N, our calculation suggests that realization of EFM is feasible with sufficient sensitivity.

It is also found from our calculation that the exchange force can be realized even with relatively large separations at 1.0<Δx<1.7. The exchange coupling is expected to be mediated through delocalized s and p electrons, which may lead to an RKKY-type oscillation. We should note that the exchange force measurements in the region (1.0<Δx<1.7) have a great advantage in that the perturbation of the approaching ferromagnetic film (tip) to magnetic moments in the other film (sample) is negligibly small. In the actual exchange-force measurements, however, we would face technical difficulties such as the jump effect when the gradient of the force exceeds the magnitude of the lever stiffness. Techniques to avoid the jump effect, as demonstrated by the recent non-contact AFM, will possibly provide the basis for RKKY-type exchange force measurements.

In conclusion, we have evaluated the exchange force between two magnetic Fe films, based on the first-principles calculations. The exchange force is sensitive to the film-film separation as well as to the surface site for Δx<1, in which the exchange force arises from the direct exchange coupling between two films. Because the magnitude of the exchange force is sufficiently larger than the force sensitivity of conventional AFM, our results suggests the possibility of constructing an EFM.

Fig. 3. The film-film separation dependence of forces in the magnetic configurations P (\( F_F \); filled circles) and AP (\( F_{AP} \); open circles), and of the exchange force defined by \( F_{ex} = F_{AP} - F_F \) (triangles) for (a) the hollow site and (b) the top site.
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References