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The effect of hydrogen adsorption on the magnetic properties of Fe adatoms on Si(001)

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Abstract

We investigate the magnetic properties for Fe adatoms on Si(001) on the basis of first-principles calculations. For the Si(001) surface, we consider systems having buckling dimers and H-terminated symmetric dimers. We find that the magnetic moment of the Fe adatom on the latter surface is larger than that of the Fe adatom on the former surface. The results positively indicate potential applications in the realization/fabrication of nanospintronics devices.

1. Introduction

Nanometre-scale structures have attracted much attention. In particular, thin films, multilayers, atom bridges, dots and small clusters composed of magnetic atoms are studied with a view to the realization of spintronics devices [1–6]. Recently, the widespread use of Si in semiconductor technology, together with new trends in microelectronics, has raised the following question—will the currently Si-based semiconductor technology be able to cope with the challenges posed by the emerging field of spin electronics? Therefore, the investigation of magnetic nanostructures on semiconductors and their interfaces is of special interest [7–9]. In the case of Fe thin films grown on Si(001)-(2×1) surfaces, the magnetization sets in at 3.6 monolayers (ML) at room temperature and 2.3 ML at 150 K, indicating a reduced magnetization due to silicide formation [7]. Experimental studies also showed that Si(001) monohydrogenated surfaces are stable against Fe chemical vapour deposition [9].

With atom manipulation using scanning tunnelling microscopes, it is possible to create characters, circles, stadiums and corrals with nanowires of magnetic atoms lying on the surface [10]. In this study, we investigate magnetic properties of Fe atoms on Si(001) as a first step in studying possible applications of these nanostructures. In the next section, we

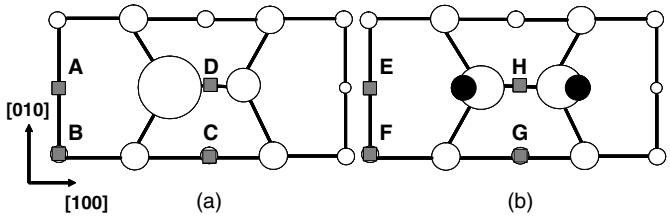

Figure 1. A top view of our model system: (a) a clean Si(001)-(2 × 1) surface and (b) an H-terminated Si(001)-(2 × 1) surface. The black circles indicate H atoms and white circles indicate Si atoms. We put an Fe adatom on the Si(001) surface at each site C and site G.

present the computational details. In section 3, we show the numerical results. In the last section, we summarize the results.

2. Computational details

In this study, the Fe adatom on the Si(001) surface system is modelled using a slab geometry with each supercell consisting of five layers of Si atoms [11] with a lattice constant equal to 5.43 Å and separated by a vacuum region (24.3 Å). We also confirmed the bulk-like local density of states of the Si atom in the fourth Si layer. Each Si layer has two atoms in (2 × 1) periodicity. The bottom layer Si is terminated by an H atom to simulate the bulk-like atomic state. We consider the following two structures: clean Si(001)-(2 × 1) surfaces and H-terminated Si(001)-(2 × 1) surfaces, as shown in figure 1. The atomic position of the upper four Si layers and the two H atoms on the Si surface are allowed to relax, while the atomic position of the lowest Si layer and bottom H layer are kept fixed. We calculated the total energy for the case of an Fe atom adsorbed on A, B, C, D sites of the clean Si(001) and on E, F, G, H sites of the H-terminated Si(001) indicated in figure 1, and found that the C and G sites are the most stable Fe adsorption sites in each of the Si surfaces. The energy difference from that of site C is 0.7 eV for the A site, 1.2 eV for the B site and 1.9 eV for the D site, and from that of the site G is 0.6 eV for the E site, 1.6 eV for the F site and 2.3 eV for the H site. Here, we present the results for Fe atoms adsorbed on sites C and G. We vary the distance between the Fe adatom and the Si(001) surface.

The calculations for the Fe adatom on Si(001) are based on the density functional theory, using the generalized gradient approximation (GGA) for the exchange–correlation energy [12]. Calculations are carried out with the plane wave and pseudopotential code [13]. The ion cores of atoms are represented using an ultrasoft pseudopotential scheme, in which the 3d states are included as valence states in the calculations. The nonlinear core correction is employed, where the core radii r_0 are 0.7 Bohr for Fe atoms and 1.5 Bohr for Si atoms. The plane wave set is cut off at a kinetic energy of 35 Ryd. We use six special k-points to sample the two-dimensional Brillouin zone. We confirmed that the numerical results converged with respect to the number of k-points and the cut-off energy used, as shown in figure 2. All numerical results are obtained from spin polarized GGA calculations with the initial magnetic moment of 2.0 μ_B/atom for the Fe atom.

3. Results and discussion

In figure 3, we show the total energy and magnetic moment of Fe atoms as a function of the distance between the Fe atom and Si surface. We define the position of the Si surface as that

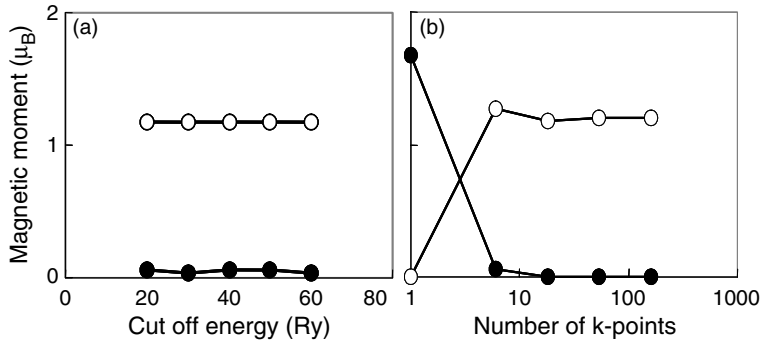

Figure 2. The magnetic moment in the supercell with the relaxed atomic configuration as a function of the cut-off energy for a plane wave set (a) and a number of k-points (b). We can see the converged results with 35 Ryd for the plane wave cut-off and six k-points for sampling the two-dimensional Brillouin zone.

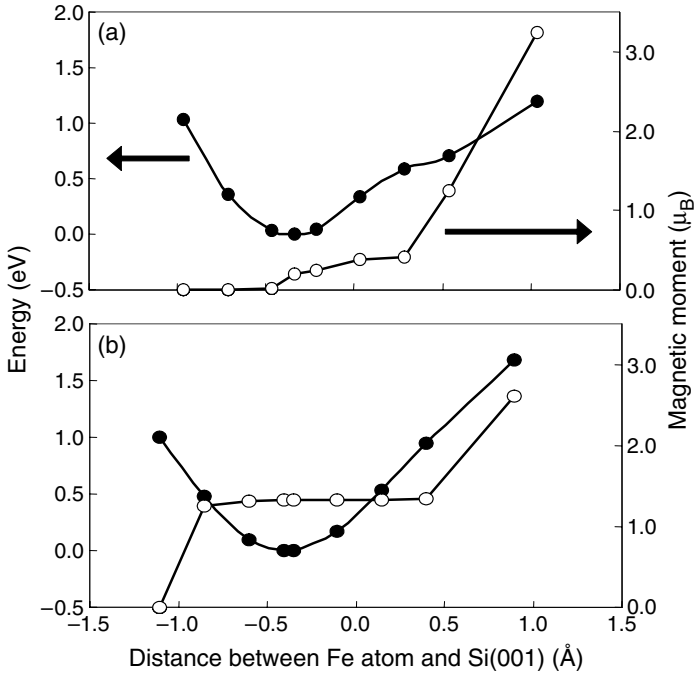

Figure 3. Total energies and the magnetic moment in the supercell as a function of the distance between the Fe adatom and the Si(001) surface in the case of the clean Si(001)-(2 × 1) surface (a) and the H-terminated surface (b). The energy origins correspond to the energy where the distance between the Fe atom and Si surface is −0.37 Å for the clean Si(001) system and −0.30 Å for the H-terminated Si(001) system, respectively.

of the topmost Si atomic centre in an ideal Si(001) 1 × 1 surface. We find energy minima at −0.37 Å for the clean Si(001) system and at −0.30 Å for the H-terminated Si(001) system. By performing the calculation with the Fe atom relaxed in plane for this atomic configuration, we find that the Fe atom does not move any more. The corresponding formation energies are 6.7 eV for the clean Si(001) and 6.5 eV for the H-terminated Si(001). H atoms adsorbed on

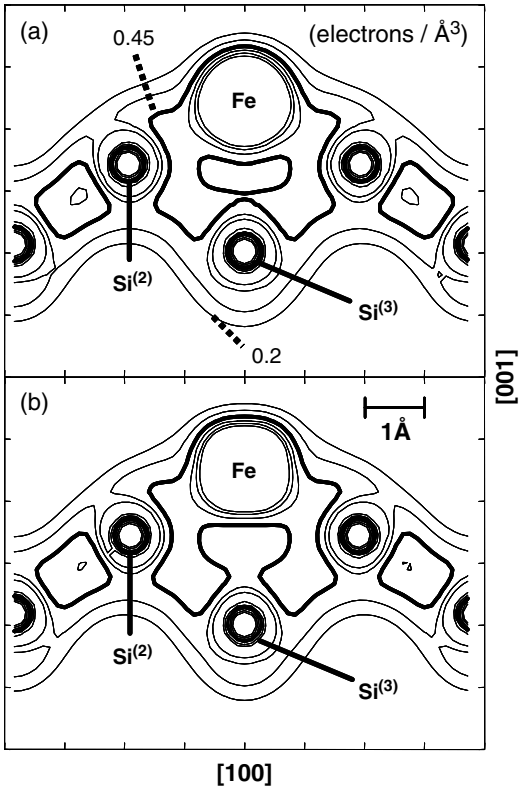

Figure 4. A contour plot of the valence electron charge density distribution in side view for the case of the Fe adsorbed on the clean Si(001) (a) and on the H-terminated Si(001) (b). Si(2) and Si(3) denote the second Si layer and the third Si layer, respectively.

Si atoms prevent the Fe atoms from penetrating the Si surface. The magnetic moment of the Fe atom for the clean Si(001) system becomes negligible. On the other hand, the Fe atom on the H-terminated Si(001) system persists. The reason is as follows. The corresponding charge density distributions in the stable structures are shown in figure 4. Since the distance between Fe and Si atoms in the third layer for the H-terminated Si(001) system is larger than that for the clean Si(001) system, the number of Fe–Si bonds, which suppress the magnetic moment of Fe atoms, for the H-terminated Si(001) system is smaller than that for the clean Si(001) system.

4. Summary

We investigated the magnetic properties of Fe adatoms on clean Si(001) and on H-terminated Si(001). Although the Fe atom on the clean Si(001) does not exhibit spin polarization, that on the H-terminated surface does exhibit spin polarization. In view of these results, we think that the nanostructures, for example, nanowires on the H-terminated Si(001), can be spin polarized and applicable in nanospintronics devices for the transport of spin polarized current. We are currently performing calculations for Fe nanowires on H-terminated Si(001).

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