Fe nanostructures stabilized by long-range interactions on Cu(111): kinetic Monte Carlo simulations

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Abstract. The magnetic Fe nanostructures formed on a Cu(111) surface were simulated by the kinetic Monte Carlo (kMC) method, in which the substrate-mediated long-range interactions between Fe adatoms are involved. The dependence of coverage and temperature on the formation of local nanostructures was investigated to reveal the microprocess of Fe nanostructures formed on a Cu(111) substrate. The simulation results show that the long-range interactions between Fe adatoms lead first to the formation of short linear chains and then to locally ordered nanostructures when they become steady at low coverages between 10 and 18 K. Based on the analysis of the formation mechanism of the Fe superlattice, it is found that the size of the repulsive ring, the distance to the first minimum potential and the diffusion barrier are the important parameters for Fe adatoms to form a superlattice on the Cu(111) surface.

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1. Introduction

Magnetic nanostructures deposited on metal surfaces are of great importance for the development of advanced atomic scale magnetic devices. The control and manipulation of magnetism and structures on the atomic scale, by scanning tunneling microscopy (STM) [1, 2] or self-assembly [3, 4], is an ongoing challenge of material science. Recent studies have indicated that the long-range indirect interactions between adsorbates [5], which come from surface-state electrons of noble metals, can be exploited to create nanostructures [6]–[12] on a metal surface.

Several theoretical studies have demonstrated that indirect adsorbate interactions can affect atomic motion and growth processes despite the fact that they are relatively small. For example, the results of a combined density functional theory (DFT) and kinetic Monte Carlo (kMC) study by Fichthorn and Scheffler [13] have shown that the long-range interactions between Ag adatoms on a strained Ag(111) surface are comparable to the diffusion barrier, and can significantly influence surface diffusion and the growth morphology in a thin-film epitaxy. The DFT and kMC calculations of Bogicevic et al [14, 15] have revealed a large increase in island density when the long-range interactions are taken into account. The theoretical studies of Fichthorn et al [16] have predicted that the repulsive part of long-range interactions inhibit island growth and lead to monodisperse islands formed early in the deposition process.

Experiments performed by STM have been able to observe nanostructures on Cu(111) and Ag(111) surfaces. For example, Repp et al [6] presented the first quantitative measurement of the long-range interactions between two Cu adatoms on a Cu(111) surface, and found local hexagonal structures with interatomic distance corresponding to the first minimum potential B (see figure 1). Knorr et al [7] examined three different metal/metal systems, and proposed that nanostructures separated with the first minimum potential might form at low temperatures. Silly et al [8, 9] discovered that Ce adatoms form a well-ordered hexagonal superlattice on an Ag(111) surface with a lattice constant of 32 Å. The self-organization of the superlattice can be attributed to the long-range interactions between Ce adatoms. These conclusions were further verified by kMC simulation recently [17, 18].
Figure 1. Long-range interactions between two Fe adatoms on a Cu(111) surface with different separations. The interaction energy is oscillatory between repulsive and attractive. The three supreme barriers $A = 32.2\, \text{meV}$, $B = -1.80\, \text{meV}$ and $C = 0.57\, \text{meV}$ are at a distance of about 5, 12.5 and 19 Å, respectively. These values were obtained from [10]. The inset shows the interactions at a larger separation based on the theory of Hyldgaard and Persson [19].

However, there are few reports on the self-organization of a superlattice by long-range interactions, especially on a magnetic superlattice. Furthermore, the intrinsic relationship between the superlattice and the long-range interactions is not well understood and needs further investigation. In the present work, the self-organization of Fe nanostructures on a Cu(111) surface by long-range interactions is systematically investigated by kMC simulation. The dependence of coverage and temperature on the shape of Fe nanostructures on a Cu(111) surface and the important parameters that affect the formation of a superlattice on a metal surface are discussed in detail. Based on the above studies, a good understanding of the relationship between the superlattice and the long-range interactions is obtained.

2. The kMC simulation model

To investigate the effect of long-range interactions on the self-organization of Fe adatoms on a Cu(111) surface, a kMC model is employed, incorporating the interaction energy $V(r)$ between two Fe adatoms shown in figure 1. The interaction energy oscillates with a period of $\lambda_F/2$, where $\lambda_F = 29\, \text{Å}$ is the surface-state Fermi wavelength of the Cu(111) surface, and decays as $1/r^2$ when the distance is larger than 20 Å, as depicted in equation (1) [19]:

$$E_{\text{int}}(r) = -AE_0 \left( \frac{2 \sin \delta_0}{\pi} \right)^2 \sin(2k_Fr + 2\delta_0) \left( k_Fr \right)^2,$$  

(1)
Figure 2. Schematic illustration of a Cu(111) surface and the diffusion path of Fe adatoms on the Cu(111) surface. The big white circles denote the Cu(111) surface, the big black circle shows the position of one Fe adatom and the small circles indicate possible positions of a second Fe adatom. All black atoms are at fcc sites, while the gray atoms are at hcp sites. Fe adatoms can diffuse along the small atoms path.

where $A$ is the scattering amplitude; $E_0$ is the surface-state band edge relative to the Fermi energy; $\delta_0$ is the phase shift; and $k_F$ is the Fermi surface wave vector. The potential for the distance $r < 20\,\text{Å}$ is described according to the values calculated by Stepanyuk et al [10]. At a distance of between 5 and 10 Å, the repulsive potential will prevent the adatoms from getting close to each other to become dimers. The corresponding maximum repulsive barrier $A = 32.2\,\text{meV}$ is at about 5 Å, and the adatoms will not be able to easily overcome it at a low temperature. The potential well between 10 and 16 Å is attractive, and the first minimum potential $B = -1.80\,\text{meV}$ is at about 12.5 Å, corresponding to the relatively stable distance between Fe adatoms on the Cu(111) surface. The second maximum repulsive barrier $C = 0.57\,\text{meV}$ at about 19 Å is considerably smaller than the barrier $A$, and adatoms will be able to easily overcome it even at a low temperature. The interactions between more than two adatoms are described by pairwise summation [20, 21].

The Cu(111) surface and the diffusion path of Fe adatoms on the Cu(111) surface are shown in figure 2. On the Cu(111) surface there are two non-equivalent adsorption sites, which are called fcc sites (black atoms) and hcp sites (gray atoms). Each adsorption site has three nearest neighbors of different kinds located at a distance $2.56/\sqrt{3}\,\text{Å}$, and the distance between sites of the same kind is $2.56\,\text{Å}$, which is the lattice constant of the Cu(111) surface. Adatoms can only diffuse from the current fcc (hcp) site to one of the nearest empty hcp (fcc) sites at a low temperature. The diffusion rate of adatoms is determined by the Boltzmann factor:

$$v_{i,j} = v_0 \exp \left( -\frac{E_{i,j}}{k_B T} \right),$$

where $v_0 = 10^{12}\,\text{s}^{-1}$ is the attempt frequency [13, 20]; $E_{i,j}$ is the activation energy between site $i$ and site $j$; and $k_B$ is the Boltzmann constant. $E_{i,j}$ consists of two parts: (i) The vertical interaction between the adatoms and the substrate $E_d$, which is the barrier for an isolated Fe monomer to diffusion from one site to the nearest neighbor on a clean Cu(111) surface. In the present work, $E_d$ is set to be 25 meV [22], and the energy difference between fcc sites and hcp sites is neglected. (ii) The lateral long-range interactions between adatoms, which comes from
a sum of pair interactions with all other Fe adatoms in the same submonolayer up to a cutoff distance $r_{\text{cut}} = 50\,\text{Å}$, as shown in figure 1. The long-range interactions are described as $E_{i(j)}$ if an adatom is at site $i$ ($j$), and the additional barrier between $i$ and $j$ is set to $0.5 \times (E_j - E_i)$. Therefore, the influence of the long-range interactions is included in the activation energy with the following form [13]:

$$E_{i-j} = E_d + 0.5(E_j - E_i).$$

(3)

The magnetic interactions between Fe adatoms are neglected, for they are much weaker when compared with the long-range interactions [10]. If the number of Fe adatoms on the substrate is equal to $N$, $3N$ different diffusions with the rates $v_1, v_2, v_3, \ldots, v_{3N}$ are possible (if one neighbor of the $i$th adatom is occupied, the rates $v_{3i-2}, v_{3i-1}$ and $v_{3i}$ are set to zero). The event of deposition or diffusion is determined by comparing a random number $\xi_1$ in the interval $[0,1)$ with $p = V_d/(V_d + R_h)$, where $V_d$ is the deposition rate and $R_h = \sum_{i=1}^{3N} v_i$ is the total diffusion rate of all adatoms. If $\xi_1 < p$, the event of deposition is chosen, and a new Fe atom is deposited on the Cu(111) substrate. Otherwise, the diffusion event is chosen. The diffusion event $m$ takes place according to the following equation:

$$\sum_{i=1}^{m-1} v_i < \xi_2 R_h \leq \sum_{i=1}^{m} v_i,$$

(4)

where $\xi_2$ is another randomly distributed number between 0 and 1. After moving the selected adatom to the new site, the distribution of potential energy near the diffused adatom is updated. The time interval between two steps is calculated according to the Poisson distribution [23]:

$$\tau = -\frac{\ln \xi_3}{\sum_{i=1}^{3N} v_i},$$

(5)

where $\xi_3$ is also a random number between 0 and 1. To avoid the influence of the finite size of the substrate, periodic boundary conditions are used when adatoms diffuse to the boundaries.

3. Simulation results of Fe/Cu(111)

3.1. Coverage dependence

The surface morphology of Fe adatoms at different coverages on the Cu(111) surface in the early period and in relatively stable states is presented in figures 3(a)–(f) and (g)–(l), respectively. The deposition flux is fixed at $F = 0.01\,\text{ML s}^{-1}$ (i.e. monolayer per second) until a desired coverage is reached, and the substrate temperature is kept at $T = 10\,\text{K}$. The size of the simulation cell is $256\,\text{Å} \times 256\,\text{Å}$, which means $100 \times 100$ adatoms in a complete submonolayer. If the coverage is $\theta$, there are $\theta \times 100 \times 100$ Fe adatoms on the Cu(111) surface.

The surface coverages in figures 3(a)–(f) are 0.005, 0.01, 0.02, 0.03, 0.04, and 0.05 ML in the early period, respectively. As shown in figures 3(a) and (b), linear short chains form, which is in good agreement with experimental observations in the Co/Cu(111) system [7, 24] and the corresponding simulation results obtained by the kMC method in the Ce/Ag(111) and Co/Cu(111) systems [25]. At a low coverage, the distance between adatoms is large and most of the adatoms are monomers, which can diffuse on the Cu(111) surface and overcome the second maximum repulsive barrier C easily. Therefore, an adatom far away might diffuse to the end.
Figure 3. Surface morphology of Fe adatoms on the Cu(111) surface obtained from kMC simulation at 10 K, with the deposition flux $F = 0.01 \text{ ML s}^{-1}$. (a)–(f) The morphology at the early period with a coverage of 0.005, 0.01, 0.02, 0.03, 0.04 and 0.05 ML, respectively. (g)–(l) The corresponding morphology when the systems are stable. The black dots represent dimers or small islands formed immediately after deposition.

of another two adatoms and form a three-atom chain. Similarly, other faraway adatoms will connect to the end of the chain in the same way. Hence, chains are the metastable structures in the self-organization at the early period, for most adatoms are in the potential well of other adatoms. However, the number of short chains increases and the morphology becomes
Figure 4. The nearest-neighbor separations between Fe adatoms with a coverage of 0.005 ML (a) and 0.05 ML (b). The dashed lines represent the distribution of the exactly deposited states and the bars are the distribution when the systems are stable.

confused with increasing numbers of Fe adatoms, as shown in figures 3(c)–(f). A few minutes later, locally ordered nanostructures form with a distance corresponding to the first minimum potential at about 12.5 Å, as shown in figures 3(g)–(k). These local nanostructures are separated by vacancies and black dots, which are made up of dimers or small islands (we call them dimers later) that are unmovable and fixed at the deposited positions at low temperatures. It is indicated that monomers can diffuse on the Cu(111) surface and rearrange to ordered structures, which are more stable than the short chains according to the long-range interactions.

Figures 4(a) and (b) show the nearest-neighbor separations of Fe adatoms at 10 K with a coverage of 0.005 and 0.05 ML, respectively. The nearest-neighbor separations are calculated as suggested by Knorr et al [7], in which the distance $r$ from a selected adatom to the nearby adatom is counted only if no third adatom is closer than it. A full width at half maximum (FWHM) for the adatoms distribution on the Cu(111) surface is used to denote the regularity of Fe adatom morphology. Therefore, the smaller the value of FWHM is, the more ordered structure forms on the Cu(111) surface. The dashed lines in figure 4 are the exactly deposited situation in which atoms are randomly distributed, while the bars are the situation when systems are stable. It is obvious that the FWHM for the dashed line (about 24.5 Å) is much larger than that of the corresponding bars (about 3.7 Å) in figure 4(a), which indicates that the ordered structures form when the system becomes stable, while the distribution of Fe atoms exactly deposited on the Cu(111) surface is random. The peaks of the bar at 2.56 Å correspond to the equilibrium distances that form ordinary dimers with chemical bonds, and the number of dimers sensitively depends on the coverage (see figure 5). Furthermore, there is a high peak at about 12.5 Å (about 65%) and a low peak at about 26 Å (about 5.4%) in figure 4(a), which correspond to the distance of the first and second minimum potentials for Fe adatoms on the Cu(111) surface. Obviously, the long-range interactions are the driving force for the formation of Fe nanostructures on the Cu(111) surface. Generally, the deposited atoms can diffuse thermally on the surface until they are captured by other adatoms, or islands present on the surface. However, if the long-range interactions are considered, the barrier between 5 and 10 Å repulses them.
Apart and prevents dimer formation when two adatoms become close. Meanwhile, if an atom is deposited far away from other adatoms, it may overcome the repulsive barrier between 16 and 24 Å even at very low temperatures and diffuse to the more stable positions, that is, the relatively stable position B at a distance of 12.5 Å.

It is also shown in figure 4(b) that the FWHM of the stable state and the exactly deposited situation is similar, while the position of the peak for the bars (at about 10 Å) is larger than that of the dashed line. This difference is also attributed to the long-range interactions for the stable state. Compared with the bars of 0.005 ML, it is found that the first peak shifts to about 10 Å, and the second peak disappears. It is well known that the average separations between adatoms are determined by the equilibrium between the repulsion and dispersion interactions. If the coverage is larger than 0.048 ML (the saturated coverage to form large-scale nanostructures with the distance equal to the first minimum potential in the Fe/Cu(111)), there is not enough space for Fe adatoms to diffuse to the most stable sites. Correspondingly, the additional Fe adatoms have to ‘climb-up’ the inner potential well and reduce the adatom–adatom separation to look for a relatively stable state. Similar phenomena have also been obtained in Ce/Ag(111) [9] and Ir/Cu(111) [26] experiments, in which the spacing between the nearest adatoms is subtly dependent on the coverage after saturation. Therefore, it is feasible to form ferromagnetic or antiferromagnetic atom pairs at different separations by changing the coverage of the adatoms.

3.2. Temperature dependence

Apart from the dependence on the coverage, the self-organization of local nanostructures is also sensitive to the substrate temperature. The lowest temperature that satisfies the self-organization process of Fe adatoms on the Cu(111) surface is 10 K, which is determined by the average diffusion rate $v_d$ (one hop per second) of a single adatom on a clean surface. With increasing temperature, the thermal activation becomes easy, and the nanostructures obtained above will be destroyed at about 18 K. When the temperature is up to 22 K, adatoms can...
overcome the largest repulsive barrier A to form dimers. Therefore, there is only a small temperature window (between 10 and 18 K) where Fe adatoms on the Cu(111) surface will self-organize into ordered nanostructures.

4. The parameters that influence the formation of a superlattice

4.1. The size of the repulsive ring

The percentage of the Fe adatoms in dimers at different coverages is shown in figure 5, in which the dots are the simulation data and the line is regressed by the dots. Figure 5 shows that the percentage of Fe adatoms in dimers increases linearly with the increase of coverage. About 96% of the Fe adatoms are monomers at a coverage of 0.005 ML. They can diffuse freely on the Cu(111) surface according to long-range interactions to look for the most stable positions and self-organize to local nanostructures. However, when the coverage increases to 0.05 ML, about 46% of the adatoms are dimers, which remain at the deposited position due to the relatively large diffusion barriers. The monomers adjust their positions around the dimers to look for stable positions, and locally ordered nanostructures are destroyed near dimers as shown in figures 3(k) and (l).

In order to reveal the formation mechanism of dimers, the steps before an adatom contacts other adatoms or small islands are registered. It is found that the steps for one adatom in all dimers are less than three, which means that all the dimers form immediately after deposition, instead of overcoming the repulsive barrier A at the temperature concerned. We define a repulsive ring as that around each adatom with a radius equal to the distance of the largest repulsive barrier. Atoms deposited within the repulsive ring of other adatoms will slip to the adatoms spontaneously and form dimers. Based on the above analysis, it can be deduced that the larger the size of the repulsive ring, the more dimers form. Therefore, the size of the repulsive ring is one of the important parameters for the percentage of adatoms in dimers and the corresponding large-scale nanostructures.

4.2. The distance of the first minimum potential

In order to further reveal the influence of the dimers on the self-organization of large-scale nanostructures, it is supposed that Fe atoms deposited inside the repulsive ring of other adatoms might be cancelled, which ensures that all the deposited atoms are monomers on the Cu(111) surface. The coverage is set to 0.048 ML and other conditions are the same as before. In this situation, all the Fe adatoms can diffuse freely to find the most stable positions. It is very interesting to find that the Fe adatoms form a large-scale ordered hexagonal superlattice on the Cu(111) surface when the system is stable, as shown in figure 6. The distance between the nearest Fe adatoms is about 12.5 Å, which is in good agreement with the position of the first minimum in the interaction potential for Fe on the Cu(111) surface. The hexagonal structures have also been proved to be the most stable configuration by Stepanyuk et al [10] due to the stabilization of surface-state electrons. In addition, similar results have been observed in recent experiments, in which Ce atoms form a hexagonal superlattice on Ag(111) at a coverage of 0.01 ML at 3.9 K [8, 9]. The main differences between the systems of Ce/Ag(111) and Fe/Cu(111) are the surface-state Fermi wavelength $\lambda_F$ and the distance of the first minimum potential. The larger the distance of the first minimum potential, the smaller the saturated
Figure 6. Superlattice of Fe adatoms on a Cu(111) surface from kMC simulation, in which atoms deposited within the repulsive ring of other adatoms are cancelled. The temperature is 10 K, the deposition flux is $0.01 \text{ ML s}^{-1}$ and the coverage is 0.048 ML.

coverage needed to form a large-scale superlattice. In this work, the saturated coverage for Fe/Cu(111) is 0.048 ML, which is much more than that for Ce/Ag(111) (0.01 ML). As indicated in the simulation results above, about 45% of the adatoms become coalescent with other adatoms and the local nanostructures are destroyed when the coverage is up to 0.048 ML. Therefore, the distance of the first minimum potential is another important parameter affecting the formation of a large-scale superlattice. It is reasonably concluded that substrates with a large surface-state Fermi wavelength and a large first minimum distance, such as the Ag(111) surface [8, 9] or Co adatoms on the 2CoML/Cu(111) surface as reported in the literature [27], will be able to form a large-scale superlattice.

4.3. The diffusion barrier

In addition, the diffusion barrier is another important parameter for the formation of a superlattice. The larger the diffusion barrier, the higher the temperature required for adatoms to diffuse. If the diffusion barrier is raised to 50 meV in the present work, the temperature needed for a single Fe adatom to hop on the Cu(111) surface is 20 K, supposing that other conditions are the same as before. It is found that the arrangement of the Fe adatoms would not be as regular as the former results. This is because the long-range interactions are much weaker compared with the diffusion barrier and the probability of an atom hopping to the more stable positions decreases with increasing temperature, as reported for Co/Ag(111) [7]. Therefore, the systems with a low diffusion barrier will easily form a large-scale superlattice through long-range interactions.
5. Conclusion

The self-organization of magnetic Fe nanostructures on a Cu(111) surface was investigated using the kMC method, in which the long-range interactions are involved. The simulation results indicate that the surface morphologies depend dramatically on the coverage and the substrate temperature. Fe adatoms deposited on the Cu(111) surface first form short linear chains and then rearrange to locally ordered nanostructures with a distance corresponding to the first minimum potential at about 12.5 Å when they become steady at low coverages between 10 and 18 K. When the coverage is up to 0.05 ML, the distance between the nearest Fe adatoms in the ordered nanostructures decreases. Based on analysis of the formation mechanism of the Fe superlattice, it is found that the existence of the dimers is unfavorable for the formation of the superlattice, and a system with a small repulsive ring, a large distance of the first minimum potential and a relatively small diffusion barrier will be amenable to forming the large-scale superlattice. The simulation results in the present work might be instructive for researchers to find magnetic nanostructures combined with advanced techniques such as spin-polarized STM, and also to find an appropriate system to form a large-scale superlattice on a metal surface through self-assembling methods for the development of advanced atomic scale magnetic devices.

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