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Ab initio study of microscopic processes in the growth of Co on Cu(001)

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ABSTRACT Using density-functional theory we investigate the energetics of various diffusion processes relevant for the heteroepitaxial growth of Co on Cu(001). We focus on how the barrier height depends on the local coordination, the interaction with the substrate and spin-polarization. We determine the temperature at which the different atomistic processes are activated and discuss their implications for the growth morphology. In particular, atomic exchange divides the temperature scale into two distinct regions: At lower temperatures growth proceeds similar to the homoepitaxial case, above the activation temperature of exchange a qualitatively different bimodal surface morphology evolves.

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1 Introduction

In order to control the fabrication of nanometer scale magnetic islands and heterostructures like Co/Cu multilayers, one needs a reliable prediction of the surface morphology for a given set of growth conditions (temperature, deposition flux). This implies knowledge of the microscopic processes active in a given temperature range and the rates at which they take place. The rate is defined as $D = D_0 e^{-E_d/k_B T}$, where D_0 is the so-called prefactor, E_d the activation energy of the process, T the temperature and k_B the Boltzmann constant.

Activation energies can be obtained from island density measurements applying the scaling relationship from standard nucleation theory (SNT) [1], which predicts that the logarithm of the island density n_x depends linearly on $1/T$. This approach has been particularly successful for systems where islands are formed by adatoms hopping on the surface [2]. However, in the growth of a heteroepitaxial system, deposited atoms may not only move on the surface but tend to replace substrate atoms in the surface layer. An example for such a system is Co on Cu(001) [3, 4]. Kinetic Monte

Carlo simulations based on input from density-functional theory (DFT) calculations of the initial growth of Co on Cu(001) show that the activation of exchange leads to a non-monotonic Arrhenius behavior of n_x and found that the concepts of standard nucleation theory are only applicable below the activation temperature of exchange [5]. On the other hand, for Co on Cu(001) quantitative information on diffusion barriers from direct methods like field ion microscopy (FIM) or variable temperature scanning tunneling microscopy (STM) is not available.

In such cases, where experimental data is lacking, it becomes even more important to provide accurate information on the processes on a microscopic level from DFT calculations. This paper reports DFT-results for the diffusion barriers of different processes obtained within the generalized gradient approximation (GGA) and focuses on how the trends can be explained by the local coordination and spin-polarization. In particular, the barriers of Co for hopping and exchange on the clean Cu(001) surface, as well as hopping along [110]-Cu steps are compared to the homoepitaxial case of Cu diffusion on Cu(001). Furthermore, the effect of substitutionally adsorbed Co atoms on the mobility of Co and Cu adatoms on the surface is investigated. Based on the relative positioning of the different processes on the temperature scale, we draw conclusions about the growth mode in the homo- and heteroepitaxial case. The last section addresses processes related to the growth of Co/Cu multilayers, namely the diffusion of Co on a Co monolayer on Cu(001) as well as of Co and Cu adatoms on a Co-film on Cu(001).

2 Computational details

The energy barriers characterizing rate processes of Co and Cu adatoms on Cu(001) are obtained using DFT with the full-potential linearized augmented plane wave method (FP-LAPW) in the WIEN97 [6] implementation. For the exchange-correlation functional the generalized gradient approximation (GGA) in the parameterization of Perdew, Burke, and Ernzerhof [7] is used. The substrate is modeled by a five-monolayer (ML) thick slab. The muffin tin (MT) radius of Co adatoms ($R_{MT}^{Co} = 2.15$ Bohr) is chosen to be smaller than the one for Cu ($R_{MT}^{Cu} = 2.20$ Bohr) to avoid overlapping of MTs due to strong relaxations in some of the geometries. Diffusion processes on the clean Cu(001) surface

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are studied in a $p(3 \times 3)$ unit cell with 16 k_{\parallel} points in the Brillouin zone (BZ). The diffusion along steps is modeled in a $p(4 \times 2)$ unit cell with 10 k_{\parallel} points in the BZ. The energy cutoff of the basis set is 13.8 Ry, which provides a numerical accuracy of 0.02 eV in the surface energy of a five-ML-thick Co(001) slab [8].

The structural optimization along the diffusion path is performed with damped Newton dynamics [9]. To find the transition state in the exchange process, the reaction coordinate is selected along the [100]-direction connecting the initial state (adatom at a fourfold hollow site) with the final state (adatom at a substitutional site in the substrate). At each point along the diffusion path, the z -coordinate of the adatom and the coordinates of remaining surface atoms are relaxed. The possibility of a symmetry reducing rotational distortion at the transition state was not considered. However, we do not expect it to lead to a significantly lowering of the energy barrier.

3 Results and discussion

3.1 Adatom diffusion on the flat Cu(001)-surface

On the clean Cu(001) surface, two types of adatom diffusion mechanisms are considered: hopping between adjacent four-fold hollow sites over a bridge site (the transition state) and exchange of an adatom with a substrate atom that is ejected onto the surface. The adsorption energy along the diffusion path and a sketch of the exchange process of Co on Cu(001) are given in Fig. 1.

The values for the diffusion barriers of Co and Cu adatoms are summarized in Table 1. For Cu, the barrier for diffusion via hopping is 0.49 eV, two times lower than the barrier for the exchange process, 1.02 eV. Unlike the heteroepitaxy of Co on Cu(001), for the homoepitaxial case of Cu on Cu(001) there is abundant information on diffusion barriers both from experiment and theory. Our values are in good agreement with previous DFT-GGA results using a pseudopotential plane-waves code (PP-PW-GGA) [10], which obtained 0.52 eV and 0.96 eV, respectively. Barriers for exchange using semiempirical methods (EAM) tend to be lower than the ones obtained from DFT-calculations (0.70 eV [10]). Experimental values [11–14] lie in the range between 0.28–0.40 eV, however, give no clue about the actual diffusion mechanism.

	E_d^{Cu} (eV)	E_d^{Co} (eV)
hopping on Cu(001)	0.49	0.61 (0.92)
exchange on Cu(001)	1.02	1.00
hopping along a [110]-step	0.40	0.55 (0.72)
hopping on 1 ML Co/Cu(001)		0.75
hopping on fct Co(001)@ $a_{\parallel\text{Cu}}$	0.46	0.76
on Cu(001)- $p(3 \times 3)$ -Co		
break away from Co-sub	0.64	1.09
hopping towards Co-sub	0.55	0.60

TABLE 1 DFT-GGA diffusion energy barriers for hopping and exchange, of Cu and spin-polarized Co on the clean Cu(001)-surface, along a [110]-step, as well barriers for break away from and hopping towards a substitutionally adsorbed Co-adatom. The barrier for hopping of non-magnetic Co on Cu(001) and along a [110]-step is given in parenthesis

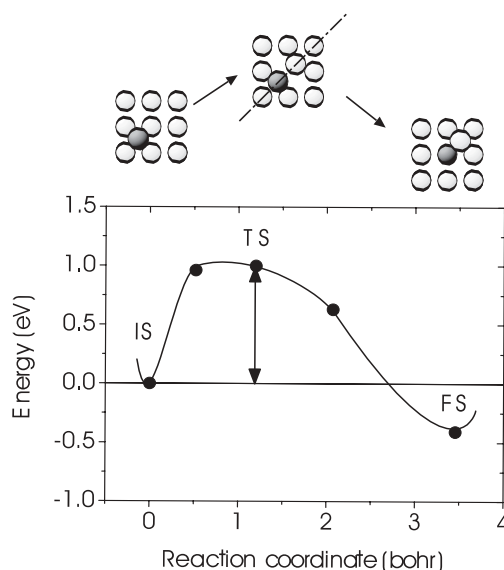


FIGURE 1 Energy along the reaction pathway for atomic exchange of Co on Cu(001). The zero of the energy is set to the energy of Co in the fourfold hollow site. The reaction coordinate represents the position of the Co atom along the [100]-direction

ism. While adatom diffusion proceeds via hopping, vacancy diffusion was proposed as a mechanism for mass transport. Boisvert and Lewis [10] obtained for vacancy diffusion a slightly lower barrier compared to the one for adatom diffusion, namely 0.42 eV from PP-PW-GGA calculations and 0.47 eV with EAM.

Considering now the heteroepitaxial case, we find that Co adatoms are less mobile than Cu, while the activation energy for exchange is similar for both species. This fact can be rationalized with a bond-cutting argument: for exchange the same type of bonds, namely Cu–Cu bonds of the ejected Cu atom, are broken in the transition state. For hopping adatom–Cu bonds are broken. Since Co–Cu bonds are stronger than Cu–Cu bonds, the barrier height for hopping of Co is higher than for Cu. This is particularly evident when considering a non-magnetic Co adatom, where the barrier for Co (0.92 eV) is almost twice as high as for Cu (0.49 eV).

Spin-polarization has a significant influence on the hopping barrier of Co: Due to the larger gain in magnetization energy at the twofold coordinated transition state compared to the fourfold initial state, the barrier is reduced from 0.92 eV (non-magnetic case) to 0.61 eV (spin-polarized case). On the other hand, the Co adatom retains a nearly fourfold coordination in the transition state of exchange and, consequently, the barrier height is not affected by spin-polarization. As indicated in Table 1 the magnetic moment of the Co adatom also shows a strong dependence on the local coordination and relaxations: It increases from $1.84 \mu_B$ to $1.94 \mu_B$ between the initial and transition state for hopping but is slightly reduced from $1.84 \mu_B$ to $1.77 \mu_B$ during the exchange process.

As mentioned above, an N -shape of island density was predicted theoretically and measured in ion-scattering experiments [5]. Applying the scaling relationship of SNT for the linear region below the onset temperature of exchange, an activation energy of 0.59 ± 0.1 eV is derived from the experimental data, which is in good agreement with the DFT-

GGA barrier for Co hopping (0.61 eV). Using a tight-binding second-moment approximation fitted to first-principles results, Stepanyuk et al. [15] obtained for Co hopping 0.66 eV, which is close to our result, while the value for exchange (0.86 eV) is somewhat lower than the DFT-GGA value.

3.2 Diffusion along steps

The equilibrium shape of islands is determined by the formation energy of different steps on the surface. On (001)-surfaces the close-packed [110]-step with a {111}-microfacet has typically a lower formation energy than the open step along the [100]-direction with a {110}-microfacet. For example in the case of Ag(001), Yu and Scheffler [16] obtained a formation energy of 0.130 eV/step atom and 0.156 eV/step atom for the [110]- and [100]-step, respectively. Consequently, in metal homoepitaxy islands nucleated on the (001)-surface have a predominant orientation along the [110]- and $[1\bar{1}0]$ -directions. We find that the formation energy of the [110]-step on Cu(001) (0.137 eV/step atom) is similar to the one for Ag(001).

During growth, adatom-step interactions and the diffusion along steps determine island shapes and step roughness. Here, we discuss the barrier for diffusion of Co and Cu adatoms along a [110]-step where the adatom moves from a fivefold coordinated adsorption site over a fourfold coordinated bridge site to the next adsorption site. We find a barrier of 0.40 eV and 0.55 eV for Cu and Co adatoms, respectively. These values are lower by 0.09 eV for Cu and 0.06 eV for Co than the respective barriers for diffusion on the bare substrate. This result can be explained by the smaller variation of the coordination between transition and initial state which is four and five at the step compared to two and four on the flat surface. This is also the reason why spin-polarization does not cause such a strong reduction of the barrier as in the case of terrace diffusion for Co. The magnetic moment of the Co adatom in the initial and bridge site at the step is $1.81 \mu_B$ and $1.88 \mu_B$, respectively (cf. Table 2).

In the case of self-diffusion of Cu a lower diffusion barrier implies that adatoms reaching a step edge can diffuse towards a kink site before a second adatom arrives at the step, thus island shapes are expected to be close to equilibrium. In the case of Co deposition the situation is more complicated: the rate for diffusion of Co along Cu-steps will be higher than on the flat surface, albeit substantially lower than the corresponding diffusion rate of Cu, therefore a certain roughening of the steps is expected. For Cu the experimental value for the barrier along the step (0.45 eV) [17] is close to the DFT-GGA result, while EAM-studies find a barrier of 0.26 eV [10, 18].

Another process, relevant in the growth of Co on Cu(001) is the diffusion of Co along the edge of a pseudomorphic Co island. For this process, Stepanyuk et al. [15] obtained a much lower value (0.31 eV) than the diffusion barrier on the flat Cu(001)-surface and found that mesoscopic strain relaxation further reduces the barrier by 0.1 eV.

3.3 Influence of substitutional Co on the hopping barrier

The substitutional adsorption of Co in the substrate layer is connected with a strong gain in energy by 0.41 eV

compared to the initial adsorption at a fourfold hollow site on the surface (cf. Fig. 1). Thus it is important to understand how the incorporated Co atoms influence the migration of adatoms on the surface. The barriers for Co and Cu adatoms to detach from a substitutional Co atom are presented in Table 1. Substitutional Co atoms hinder Cu hopping by raising the barrier by 0.15 eV beyond the bare-surface value, while Co adatoms need an additional 0.48 eV to overcome the attractive potential of substitutional Co. Thus, substitutionally adsorbed Co acts as a nucleation center for both chemical species, the effect being particularly strong for Co adatoms. On the other hand, the attraction of the substitutional site is short-ranged and the barriers for both species to hop toward this site are essentially equal to the bare-surface values. The DFT-results also show that pinned Co atoms can exchange into the surface with a barrier comparable to the one on clean Cu(001) [19]. This provides a mechanism for forming compact Co inclusions in the surface.

3.4 Onset temperature for diffusion

In this section we evaluate the onset temperature of the different processes and provide a qualitative picture of the growth mode in the homo- and heteroepitaxial case. The onset temperature T_i is defined as the temperature at which the process i takes place at least once per second, i.e., at a rate $\Gamma = 1 \text{ s}^{-1}$:

$$T_i = \frac{E_d^i}{k_B \ln(\Gamma_0/\Gamma)}. \quad (1)$$

The prefactors for hopping, exchange and diffusion along the step are set to values obtained from a molecular-dynamics study using the embedded-atom-method (MD-EAM) for Cu on Cu(001) [10], $D_0^h = 2 \times 10^{13} \text{ s}^{-1}$, $D_0^{\text{ex}} = 4.37 \times 10^{14} \text{ s}^{-1}$, and $D_0^{\text{st}} = 3 \times 10^{12} \text{ s}^{-1}$, respectively. Recent calculations with semiempirical potentials fitted to first-principles results find a prefactor of $2 \times 10^{13} \text{ s}^{-1}$ for hopping of Co on a Co island on Cu(001) [20]. This number equals D_0^h for Cu-self-diffusion reported in [10]. The MD-EAM values reflect the trend that prefactors for concerted processes like exchange are higher due to the higher number of vibrational modes in the transition state compared to the initial state.

We note that the activation temperatures displayed in Fig. 2 are only a rough estimate and the absolute values may differ by as much as 20–30 K from the ones obtained in our DFT-kMC simulation [5]. In the latter the rate of occurrence of a certain process depends on the total rate of all possible processes and in particular, on the deposition rate F : e.g its activation can be pushed to higher (lower) temperatures by increasing (reducing) F . Nevertheless, the relative order of the individual processes is in good agreement with the predictions from the DFT-kMC simulation and the experimental data. Moreover, it allows us to draw some conclusions on the growth mode comparing the homoepitaxial (Cu on Cu(001)) to the heteroepitaxial case (Co on Cu(001)).

In the homoepitaxial growth of Cu(001) adatom diffusion is expected to be activated at about 190 K. At this temperature step edge diffusion is already effective and leads to straight step edges. Breeman, Rosenfeld and Comsa [21] discussed

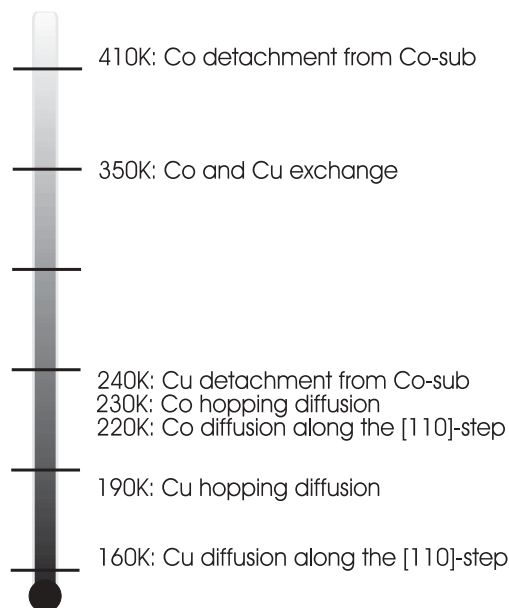


FIGURE 2 Activation temperature of the different diffusion processes of Cu and Co adatoms on Cu(001)

atomic rearrangements in islands e.g., via diffusion along island edges as a possible mechanism for island nucleation in the absence of thermal diffusion. Dürr et al. [14] observed no compact island formation in the growth of Cu on Cu(001) below 150 K. Breeman and Boerma [13] determined the onset temperature of adatom diffusion from low energy ion scattering (LEIS) measurements to be 140 K. Both findings are in good agreement with our result. Exchange diffusion does not play an important role for Cu self-diffusion because it is activated at much higher temperatures at which the rate for adatom diffusion via hopping is as much as $1.9 \times 10^7 \text{ s}^{-1}$.

For the heteroepitaxial growth of Co on Cu(001) terrace diffusion starts at higher temperatures than for Cu, namely above 230 K. In agreement with this, the intensity oscillations measured in He-scattering experiments [27] are strongly suppressed below 250 K and eventually disappear for lower temperatures, indicating a negligible thermal diffusion below 220 K. On the other hand, the exchange process both for Co and Cu is activated at 350 K. Consequently, below the activation temperature of exchange no intermixing is expected and island nucleation will very much resemble the homoepitaxial case, with the only difference that the adatoms are less mobile than in the homoepitaxial case. The activation of exchange results in a dramatic change in the surface morphology: at 350 K Cu adatoms generated by the exchange processes are able to detach easily from substitutional Co and diffuse on the surface to form large Cu islands. On the other hand, for Co the detachment process is not activated until 410 K – in the temperature range between 350–400 K the pinning of Co at substitutional Co results in a higher density of small Co-islands. Experimentally, a sudden drop in the average island separation is observed between 323 K and 365 K [27]. A bimodal growth mode with two different types of islands with respect to size and chemical composition has been found both in measurements of the island size distribution at 415 K [4] and in our DFT-kMC simulations [5].

Processes like the generation of surface vacancies at elevated temperatures may favor the substitutional incorporation of Co and thus may influence the growth mode. However, such mechanisms go beyond the scope of this work and have not been considered.

3.5 Co/Cu Multilayer growth

Co/Cu multilayers exhibit phenomena like giant magnetoresistance [22, 23] and interlayer exchange coupling [24–26]. These effects depend sensitively on the quality of the interface. During the deposition of Co on Cu(001) experimental studies reported that the second layer starts to grow before the first one is completed [29, 30]. This deviation from the layer-by-layer growth is referred to as a “bilayer” growth mode. DFT calculations showed that in thermodynamic equilibrium the formation of bilayer Co islands is energetically more favorable than the single monolayer [8]. Studying the temperature dependence of this behavior, He-scattering experiments [27, 28] found that between 240–300 K the intensity maximum corresponding to the completion of the first layer is suppressed. As an explanation, Dijken [27] suggested a higher mobility of Co on 1 ML Co/Cu(001).

To shed more light on the kinetics and the microscopic processes underlying this behavior, we studied the diffusion barrier of Co on a strained Co monolayer on Cu(001) and the barrier of Co and Cu on a 5 ML Co-film strained at the lateral lattice constant of Cu. Contrary to the suggestion of Dijken [27], Co adatoms are found to have a lower mobility on a strained Co ML on Cu(001) (0.75 eV) than on Cu(001) (0.61 eV). This result is in line with the trend that the breaking Co-Co-bonds costs more energy than the breaking of Co–Cu bonds. As shown in Table 1, the barrier for hopping of Co on 1 ML Co/Cu(001) and on a strained fct Co(001)-film is essentially the same.

On the other hand, the situation may be different on a small strain-relaxed Co-island. Indeed, Stepanyuk et al. [15] found a barrier of 0.58 eV for Co diffusing on a Co island containing 36 atoms. On the other hand, the Ehrlich–Schwoebel barrier and the edge exchange barrier are high, 1.03 eV and 1.25 eV, respectively. This implies a hindered interlayer mass transport and a higher probability for islands of the next layer to nucleate on Co-islands.

After depositing Cu on a thick Co film on Cu(001), Dijken [27] observed a reduced first maximum and a deeper first minimum in the He-scattering intensity. Dijken [27] suggested that the mobility of Cu on the cobalt film should

	IS	TS
hopping on Cu(001)	1.84	1.94
exchange on Cu(001)	1.84	1.77
hopping along a [110]-step	1.81	1.88
hopping on 1ML Co/Cu(001)	1.94	1.99
hopping on fct Co(001) _{a Cu}	1.92	1.97
break away from Co-sub	1.84	1.93

TABLE 2 Magnetic moment of the Co adatom in the initial (IS) and transition (TS) state for the diffusion processes given in Table 1

be higher than the one of Co on Cu(001) but lower than the mobility of Cu on Cu(001). The DFT-GGA calculations (cf. Table 1) find that the hopping barrier of Cu on the fct Co(001)-film (0.46 eV) is indeed lower than the barrier of Co on Cu(001) (0.61 eV) but similar to the one of Cu on Cu(001) (0.49 eV). The reasons for the reduced first maximum in the He-intensity oscillations during the deposition of copper on fct Co(001) still need further investigation.

4 Conclusion

In summary, we present DFT-GGA activation energies of various diffusion processes in the Co/Cu-heteroepitaxy and discuss their consequences on the growth morphology. Both for Co and Cu adatoms diffusion via hopping is favored over the exchange process, the barrier for exchange being 1.0 eV. Co adatoms are found to be less mobile on the Cu(001)-surface than Cu adatoms. The corresponding barriers are 0.61 eV and 0.49 eV for Co and Cu, respectively. Spin-polarization reduces the barrier for hopping of Co by 0.31 eV due to a substantial gain in magnetization energy in the lower-coordinated transition state. The barriers for diffusion along a [110]-step on Cu(001) are lower than the ones on the flat substrate. Mobility of adatoms along island edges is therefore expected even below the activation temperature for diffusion of isolated adatoms.

Based on the information on the diffusion barriers and adsorption energies, two regimes are identified in the initial growth of Co on Cu(001). Below the activation temperature of exchange a growth mode similar to the homoepitaxial case and a sharp Co/Cu-interface are expected. The activation of atomic exchange results in a dramatically different surface morphology. Substitutionally adsorbed Co atoms tend to trap Cu and Co adatoms on the surface by enhancing their barrier to diffuse away by 0.15 eV (Cu) and 0.48 eV (Co) with respect to the barrier on the bare substrate. The interplay of atomic exchange, pinning at substitutional Co and high diffusion rate of Cu atoms on the surface gives rise to a bimodal growth mode.

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