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Surface Science 381 (1997) 106–116

surface science

Strain-driven formation of two-dimensional holes on Cu(111) after the deposition of Fe

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Received 16 July 1996; accepted for publication 27 December 1996

Abstract

The formation and growth of one-monolayer-deep holes after the deposition of Fe on a Cu(111) vicinal surface at 300 K are studied by scanning tunneling microscopy (STM). At low Fe coverages, hole formation starts between separate Fe islands grown at step edges. As hole formation is accompanied by the creation of edge energy, it is assumed that the tensile stress field between the adjacent Fe islands provides the driving force for this process. At higher Fe coverages, another hole formation process is induced by the strain field at Fe wires, resulting in a step-up diffusion. Both hole-creating processes can be suppressed by depositing Fe at lower temperatures and subsequently sealing Cu steps and Fe wires by depositing Au. © 1997 Elsevier Science B.V.

Keywords: Copper; Iron; Molecular beam epitaxy; Scanning tunneling microscopy; Surface stress; Vicinal single crystal surfaces

1. Introduction

The growth of ultra-thin Fe layers on Cu substrates is of particular interest, as the magnetism of thin Fe films may depend significantly on their structural properties [1]. Fe films have mostly been studied on Cu(100) [2–5], revealing a layer-by-layer growth mode starting from the second monolayer. With increasing film thickness, the out-of-plane magnetization changes to in-plane magnetization at about the eleventh monolayer (ML), and the initial fcc phase starts to transform to the bulk bcc phase between the fifth and the eleventh ML.

The first results regarding the magnetic properties of Fe films on Cu(111) were rather contradictory [6–8]. While AES and LEED studies claimed a layer-by-layer growth at room temperature up to a thickness of 0.8 nm [9,10], an initial STM study distinctly proved a three-dimensional island formation right from the beginning, with a preferential decoration of step edges on the upper terrace [11]. As a special characteristic, the formation of two-dimensional holes of hexagonal shape has been observed on the Cu terraces, generally assumed as an Fe-induced Cu diffusion process [11]. Similar observations of hole formation have been reported for Co on Cu(111) [12], and have been explained as a Co-induced etching process resulting in the emission of surface vacancies, and thus the formation of holes. At the same time, an intermixing of Co and Cu was thought to take place, forming a dilute surface alloy [13].

The preferential decoration of steps can be utilized to fabricate quasi-one-dimensional Fe or Co

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PII S0039-6028(97)00065-4

wires on Cu(111) vicinal surfaces [14]. One may expect a considerable reduction in the magnetic moments of the magnetic wires if there is an alloying reaction involved in hole formation. To decide whether or not alloying takes place, in the present paper the hole formation process was studied in detail by STM. The experimental findings are found to be explicable by a new tensile-strain induced mechanism without alloying. In addition, experimental conditions are described which suppress the undesirable formation of holes.

2. Experimental

The experiments were performed in a multichamber facility equipped with an Fe evaporator, LEED, AES, an Ar-ion source for cleaning, and a room-temperature STM. The Cu(111) substrate was oriented 1.2° in the [112] direction, giving a mean step distance of 10 nm in the [$\bar{1}$10] direction with a (100) microfacet. The cleaning procedure comprised many cycles of Ar-ion bombardment (1–2 keV) and annealing at 700 K until impurities were below the AES detection level, with the LEED patterns revealing sharp spots of three-fold symmetry.

Fe was deposited from a wire of 99.999% purity heated by electron bombardment in a water-cooled evaporator. The ion current was used to guarantee a controlled deposition rate of typically 0.33 ML min^{-1}. In the submonolayer region, the deposition rate was determined by STM coverage measurements and checked by the layer-by-layer growth of Fe on Cu(100), also measured by STM. The grazing incidence angle of the Fe flux on the Cu substrate was fixed at 35°. The base pressure in the deposition chamber was 6×10^{-11} mbar, and rose to 2×10^{-10} mbar during Fe deposition. The usual deposition temperature was 300 K, but some experiments were also carried out at lower temperatures (down to 200 K). Immediately after deposition, the sample was transferred to the STM chamber. The STM images were recorded at a pressure of 4×10^{-11} mbar. The constant-current topographical images were taken at a typical sample bias of ± 0.1–± 0.8 V and a tunneling current of 0.5–2 nA. After each deposition experiment, the sample was cleaned, annealed and checked by the procedure outlined above.

3. Results

The clean Cu(111) vicinal surface shows nearly parallel steps in the ⟨110⟩ direction, with no indication of step bunching due to pinning centers. Locally, the nominal mean step distance of 10 nm was not maintained during the series of experiments. In the STM images, the atomic steps look frizzy due to the diffusion of atoms or kinks along the steps [15], or due to tip–surface interactions [16].

In Fig. 1, at the lowest coverage of 0.03 ML Fe deposited at 300 K, Fe islands of 1 ML in height decorate the atomic Cu steps, solely at the upper step edges [11]. As there is a lack of dynamic range of the grey-scale pictures in images with

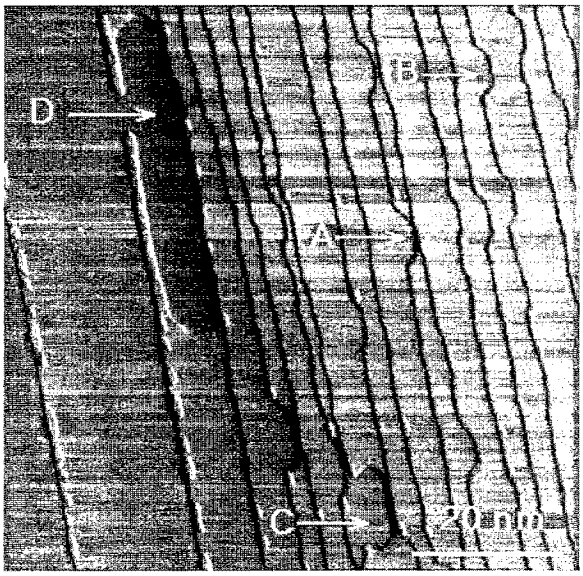


Fig. 1. STM image of 0.03 ML Fe deposited on a Cu(111) vicinal surface at 300 K. The upper Cu step edges are decorated with Fe islands of 1 ML in height. Near the Fe islands at the step edges (arrow A) or mainly between adjacent Fe islands (arrows B, C, D), an erosion starts into the ascending Cu terraces (arrows A, B) resulting in the formation of Cu holes (arrows C, D) with openings to the lower terrace. (Figs. 1, 2, 5 and 8 have all been image-processed to make the steps more clearly visible).

large variations in height, the STM images have been image-processed to suppress low-space frequencies and to locally enhance the variations in height by differentiation. The pictures suggest a landscape illuminated from the right. Owing to the high mobility of diffusing Fe adatoms on the Cu(111) terraces and the relatively low deposition rate of 0.33 ML min^{-1}, the main nucleation process takes place at the step edges. Only for large terraces of more than 20 nm in width are there also Fe islands on the flat terraces (Figs. 2–5). In contrast to the islands on steps, these are 2 ML in height. The density of Fe islands along the steps depends on the width of the Cu terraces which feed them. Therefore, the edges of large terraces are more densely decorated with Fe islands than those of narrow terraces. More details on the nucleation and growth behaviour of Fe on such vicinal Cu(111) surfaces, especially with the aim of producing quasi-one-dimensional magnetic wires, will be described in a forthcoming paper [17].

However, the most striking features of Fig. 1 are the instabilities in the originally parallel arrangement of the Cu steps. Near some individual Fe islands (arrow A), or mainly between two separated islands (arrow B), the Cu steps form a negatively curved bulge into the terrace. This process is the initial stage of the formation of open holes in the upper Cu terraces. The holes may either grow across the whole terrace (arrow C), or form extended holes between the steps (arrow D). Thereby, large amounts of Cu atoms have to diffuse out of the openings to be distributed along the Cu steps, or have to diffuse across the lower Cu terraces.

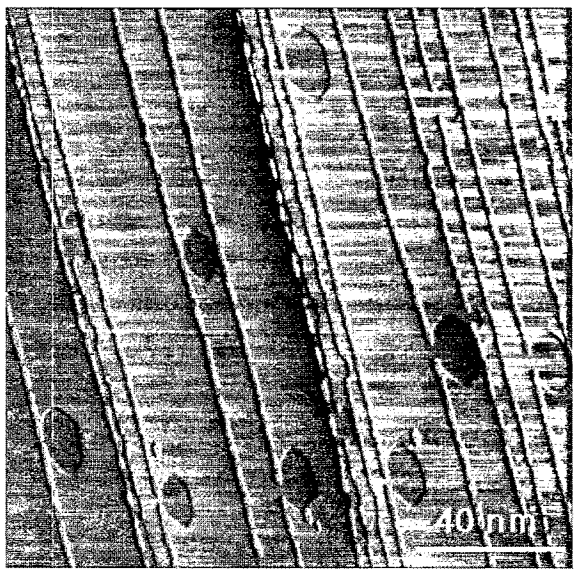


Fig. 2. STM image of 0.06 ML Fe grown on Cu(111) at 300 K. With increasing coverage the density of Fe islands along the Cu edges increases, with the widths of the hole openings decreasing. The Cu holes grow preferentially along the Fe islands, assuming an oblong shape. The size of the Cu holes does not correlate to the Fe coverages, but to the time period after deposition.

In Fig. 2, at a higher Fe coverage of 0.06 ML the Cu steps are more densely decorated. The 1 ML Fe islands begin to coalesce along the descending steps of large terraces. The probability of hole formation decreases as the separation distance of the Fe islands becomes smaller. The oblong shape of the Cu holes shows that they grow preferentially at step edges along the chains of Fe islands; this causes their oblong shape. The size of the Cu holes does not correlate with the coverage of deposited Fe, but rather with the time elapsed after deposition. Large amounts of Cu are transported out of the openings to be distributed along the originally lower terraces.

More details of the mass transport involved in hole formation are shown in Figs. 3 and 4. In Fig. 3, the Cu atoms from the right hole diffused through the opening before they spread along the descending Cu step (on the upper step edge decorated with Fe islands). Since no additional minor Cu aggregation is detectable below the Fe islands, the distribution by edge diffusion must be concluded to extend over long distances. In Fig. 3a, the amount of Cu material leaving the left hole has diffused along the Cu step; however, in the lower part of the image, it has filled the small Cu terrace between the decorating Fe islands and the Cu step (region F). Thus, the small Cu terrace has expanded to the left, forming a new double-height Cu step by enclosing the existing Fe islands at the step edge. The profile of Fig. 3b along the upper white line in Fig. 3a clearly shows the difference between the apparent heights of 0.21 nm for a 1 ML Cu step and 0.18 nm for a 1 ML Fe island at the upper step edge. The profile of Fig. 3c along

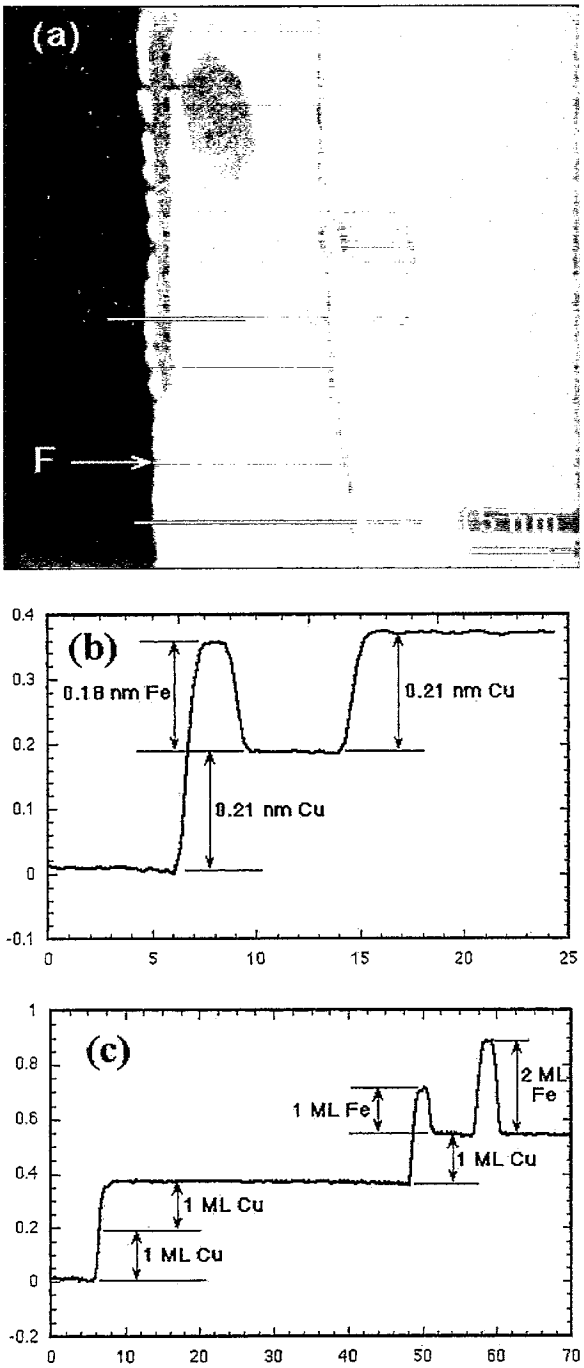


Fig. 3. (a) STM image of 0.02 ML Fe on Cu(111) grown at 300 K, illustrating the mass transport of Cu out of the holes. Cu diffuses out of the opening of the right hole before it spreads along the descending Cu step. Since there is no additional Cu aggregation along the step, long diffusion distances have to be assumed. For the left Cu hole, the same diffusion results in the filling up of the small terrace between the decorating Fe islands and the Cu step in region F. (b) Height profile along the upper line of (a), showing two Cu steps and a 1 ML Fe island at the edge. (c) Height profile along the lower line of (a) showing (from left to right) the filled-up 2 ML small Cu terrace, the larger middle Cu terrace, a 1 ML decorating Fe island, and finally a 2 ML Fe island on the terrace.

the lower white line in Fig. 3a shows a 2 ML (0.39 nm) Fe island on the right of the terrace, which on the left is followed by a 1 ML Fe island at the step edge (0.18 nm) and a large Cu terrace with a newly filled 2 ML Cu step 0.42 nm in height on the extreme left.

Diffusion out of the opening of a hole followed by distribution along the Cu steps is not the only process which occurs. The Cu atoms can also diffuse freely on the adjacent lower terrace. The small Cu terrace between the two larger terraces in the middle of Fig. 4 was originally decorated with isolated Fe islands, but the Cu atoms coming out of the opening of the hole have diffused over the small terrace before being trapped between the Fe islands, thus forming a 1 ML stripe of alternative Fe and Cu patches starting above site B and extending beyond site A. Fig. 4b proves this by the profile along the Fe–Cu stripe from A to B, showing a 2 ML Fe island on the left, then the corrugation owing to the difference of 0.03 nm in height between 1 ML Fe and Cu, and the 1 ML high drop to the small Cu terrace on the right.

The initial stage of hole formation at Cu steps not completely decorated with Fe islands has been shown, as well as their preferential growth along the steps and the diffusion of Cu material out of holes. However, it has not been illustrated *when* exactly hole formation starts and how fast it proceeds. This can be shown experimentally by performing a double deposition experiment to obtain two snapshots during the same experiment, gaining information about a time-dependent process from a single STM image.

In Fig. 5a, first 0.1 ML Fe was deposited on Cu(111) at 300 K, followed by a second deposition of 0.1 ML Fe at 300 K after a delay of 40 min. The features observed can be explained in the

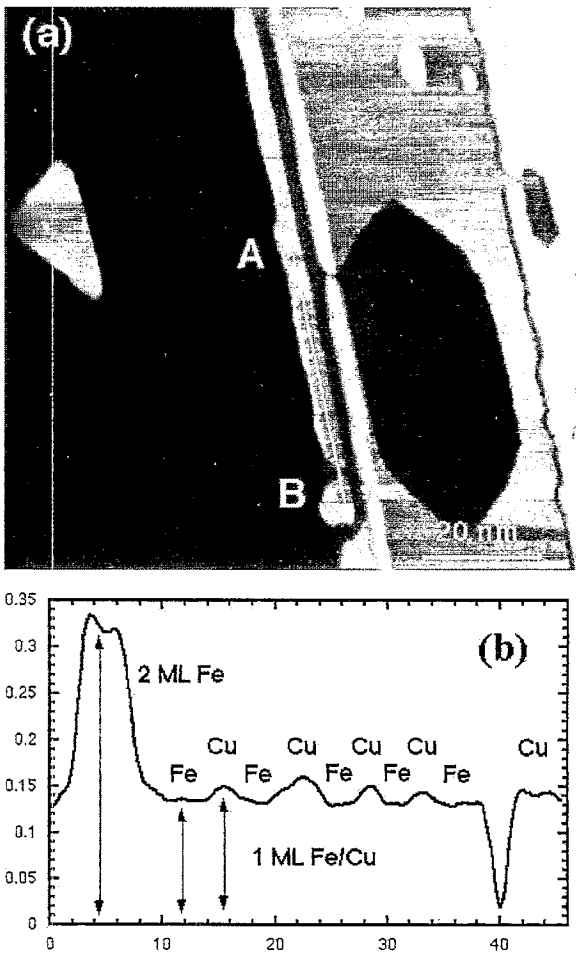


Fig. 4. (a) STM image of 0.1 ML Fe deposited on Cu(111) at 300 K. Mass transport of Cu out of the holes is by diffusion and trapping of Cu between a chain of Fe islands along the edge of a small terrace. (b) Height profile along the line from A to B in (a) showing a 2 ML feature (either 2 ML Fe or 1 ML Fe+1 ML Cu), and patches of 1 ML Fe and Cu alternating along the stripe.

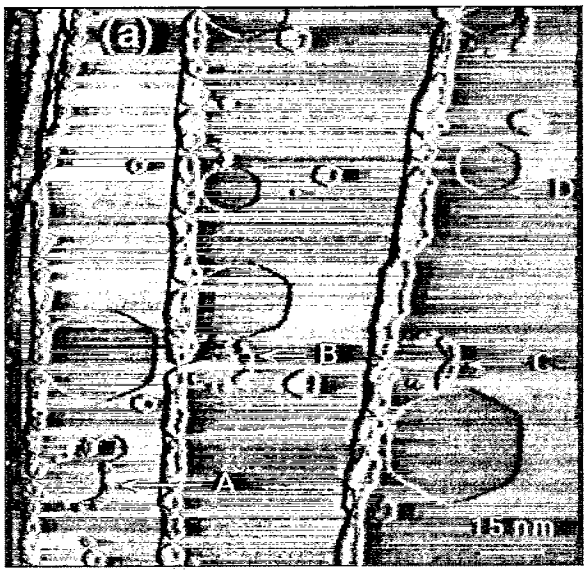
following way. During the first deposition, only the Cu steps are decorated. During the delay time of 40 min, primary holes (A, B, C) form with openings to the next descending terrace. During the second Fe deposition, the edges of these primary holes are decorated, the already existing Fe islands grow larger and larger, and coalesce along the steps. After the second Fe deposition, the formation of secondary holes starts from openings in the primary holes (A, B), or at the Cu steps (D). These secondary holes cannot be decorated with Fe. Their growth causes the primary holes to become partially (B) or completely (C) filled. The hole at D has probably filled its opening to the descending terrace itself and started to move freely over the terrace. From this double deposition experiment, it is possible to estimate the growth rate of the primary holes. After 40 min a maximum diameter of about 15 nm is attained, corresponding to a mean net diffusion flux of 1–2 atoms per second out of the holes. From this, it follows that the very slow hole formation and growth processes do not operate effectively during an Fe deposition of some 10 s, but only after it. As a conclusion drawn from this process proceeding slowly at 300 K, we intend to freeze out hole formation at slightly lower deposition temperatures.

In Fig. 5b, at a temperature of 223 K a first deposition of 0.1 ML Fe was followed by a delay of 45 min and a second deposition of 0.1 ML Fe. Then the sample was warmed to 300 K for STM observation, showing no decorated primary holes (i.e. during the delay period at 223 K, no holes have formed). All large, non-decorated holes are created after the second deposition following warming to 300 K.

These double deposition experiments proved our assumption of being able to freeze out hole formation after deposition by using lower temperatures. However, in order to also suppress hole formation during warming and STM observation at 300 K, the starting points of hole formation (i.e. the free parts at the Cu steps between the Fe islands) should be eliminated. This can be done by depositing metals like Ag or Au respectively, wetting the bottom sides of the steps and consequently sealing them against hole formation.

In Fig. 6a, the desirable step wetting was checked for 0.05 ML Ag grown on Cu(111) at 300 K. Ag preferentially decorates the bottom of Cu steps, without any nucleation taking place between the steps. There is a tendency to form stripes instead of an ideal one-dimensional wetting. The Ag stripes (1 ML in height) form a known superstructure [19,20] of a periodicity of (8×8).

In Fig. 6b, in a second run, 0.1 ML Fe was deposited. As expected, in step regions wetted with



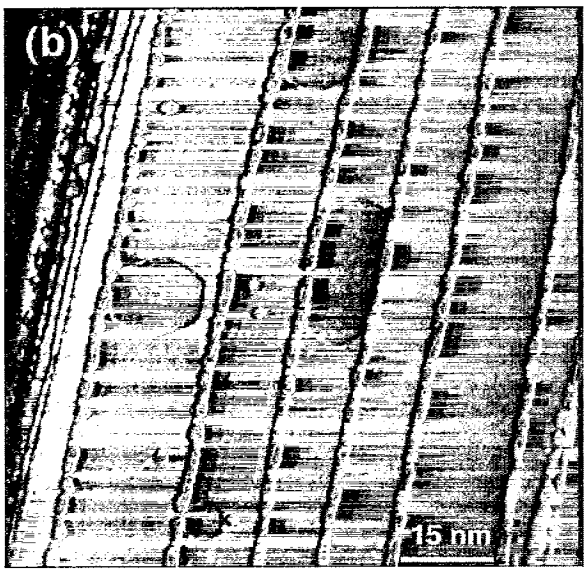
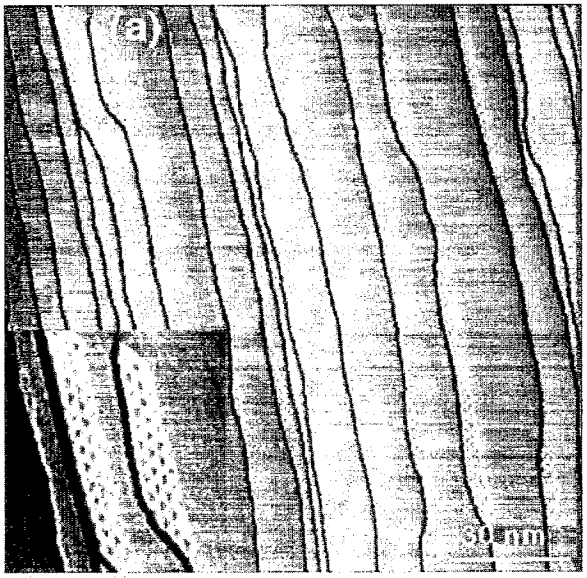


Fig. 5. (a) STM image of a double deposition of 0.1 ML Fe on Cu(111) at 300 K with a delay time of 40 min. In the first deposition, only the Cu steps are decorated. During the delay time primary holes (A, B, C) form, which are then decorated during the second deposition. Note that all non-decorated holes are formed after the second deposition. (b) A similar double deposition experiment of 0.1 ML Fe on Cu(111) at a lower temperature (223 K) with a delay time of 45 min demonstrating the freezing out of the hole-formation process. Only Cu steps are decorated (i.e. no primary holes form during the delay time at 223 K). The non-decorated holes again form after the second deposition during warming to 300 K in the STM.



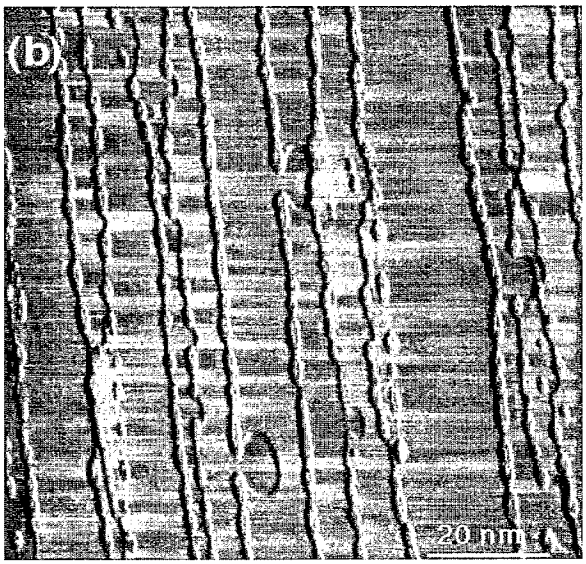


Fig. 6. (a) Nearly ideal wetting of 0.05 ML Ag along the bottom sides of Cu steps grown at 300 K. Ag forms a (8 × 8) superstructure (detail in inset). (b) Predeposition of 0.05 ML Ag followed by the deposition of 0.1 ML Fe on Cu(111) at 300 K suppresses hole formation at those steps sealed by Ag. At Ag-free steps, hole formation still continues.

Ag, hole formation was suppressed. However, in Ag-free step regions, hole formation still occurs.

The final method of suppressing hole formation is to combine the methods described above. The

deposition of Fe at lower temperatures (250–273 K) is followed by the sealing of the Cu steps by depositing 0.2 ML Ag or Au at 250–273 K.

Results have been discussed for low Fe coverages, at which the Cu steps are decorated with isolated Fe islands, leaving small parts of Cu steps in between so that hole formation can start. With increasing Fe coverage the Fe islands coalesce along the step edges, forming quasi-one-dimensional wires. Openings favouring hole formation are increasingly sealed by the coalescence of Fe islands. Fig. 7 illustrates this stage at an Fe coverage of 0.2 ML grown on Cu(111) at 300 K. Some of the Cu holes still have openings to the descending Cu terrace (A), but others (C) do not. There must be an alternative hole formation process occurring here. The origin of hole creation, however, is still in the vicinity of the Fe wires. Small holes (B) can move away from the Fe wires, across the Cu terrace.

Finally, in Fig. 8, at an Fe coverage of 0.6 ML deposited on Cu(111) at 300 K, the Cu steps are continuously decorated with 1 ML and partly with 2 ML thick stripes of Fe, leaving no openings; nevertheless, large extended holes (H) have been formed. This means that a different Fe-induced mechanism of hole formation proceeds. The growth of Cu holes is locally pinned whenever holes arrive at already existing Fe islands (see arrows in Fig. 8) [11]. The Cu material leaving the holes has to diffuse step-upwards and spread along the Fe wires.

This latter hole formation process at higher Fe submonolayer coverages can be successfully suppressed by following the above-mentioned rule of using lower deposition temperatures and sealing with Au.

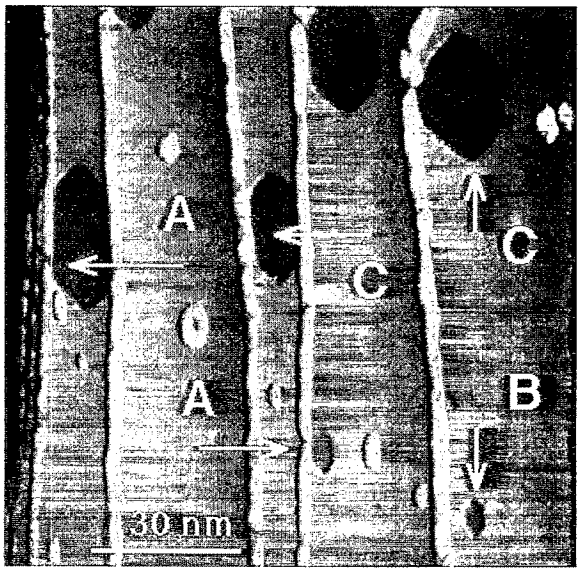


Fig. 7. With increasing coverage of 0.16 ML Fe deposited on Cu(111) at 300 K, the coalescence of Fe islands along steps starts with the formation of quasi-one-dimensional wires. Although the number of openings for holes to the next descending terraces (arrows A) is decreasing and finally vanishes, the formation of holes near the Fe wires still continues. Small holes (arrow B) can move over the terraces.

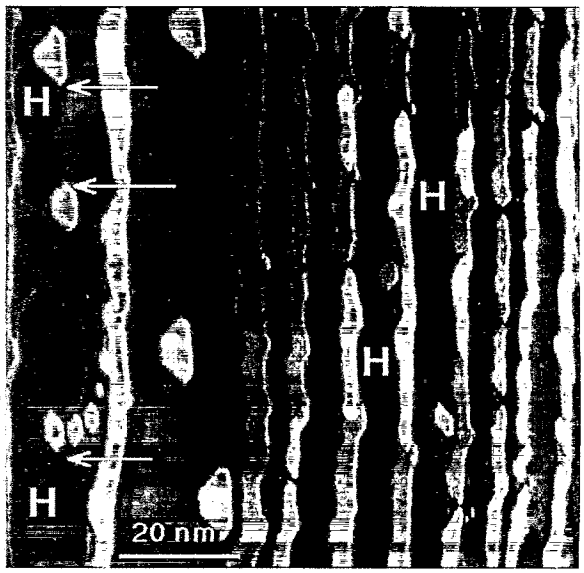


Fig. 8. At a coverage of 0.6 ML Fe grown on Cu(111) at 300 K, most Cu steps are decorated with continuous Fe wires (1–2 ML in height). A different hole-formation process without openings to descending terraces is occurring. The Cu material leaving the spreading holes between the steps (H) has to diffuse step-upwards to be distributed along the Fe wires or ascending decorated Cu steps.

4. Discussion

How can the origin and the driving force of the hole formation processes be explained? Before

discussing our new model, which is directly correlated to the existence of steps and the decoration of the step edges with Fe, we will first briefly discuss other previously published models of hole formation for the systems Fe/Cu(111) and Co/Cu(111) [11–13]. The first possible explanation of hole formation of Fe/Cu(111) being induced by Ar-ion sputtering during sample preparation was dismissed by the authors [11] because the uncovered substrate never showed such holes and pre-existing holes should be decorated with Fe islands, which was never observed. Therefore, the authors' general conclusion was [11] that the deposition of Fe atoms gives rise to the diffusion of Cu atoms by an exchange mechanism between Fe and Cu at steps, or an excitation of Cu terrace atoms during the initial Fe condensation process. Hole formation has been studied in more detail in the Co/Cu(111) system, and has been explained by a Co–Cu surface alloying, owing to the emission and diffusion of surface vacancies, which agglomerate in mobile holes [12]. Such Co-deposition induced holes also occur close to steps. A most remarkable observation was reported in a recent STM study of hole creation and motion for Co on Cu(111) and on clean Cu(111). Small holes were formed by tunneling-current pulses [13]. Holes produced on clean Cu terraces were almost completely immobile at room temperature; only in the shear stress field in the vicinity of a screw dislocation holes were displaced towards the dislocation core [13].

Summarizing the experimental observations, two important results emerge: (i) there is no distinct correlation between the Fe coverage and the hole coverage, which would be expected for an alloying process, and (ii) hole growth always starts at Cu steps, or Fe wires, proceeding continuously at 300 K with increasing time after deposition. To explain these results, a new strain-driven mechanism is proposed to be operative in the observed hole formation and growth without alloying.

In the epitaxial growth of a crystalline thin film on a crystal surface, stresses occur resulting from the misfit of different lattice constants of the same lattice type, or from the mismatch of different lattices. These stresses are assumed to be released by either a strained pseudomorphic growth of the deposit in the first few monolayers, or by the spontaneous formation of misfit dislocations if a critical deposit thickness is reached. To generalize this concept, it is also possible that part of the stress is transferred to the uppermost layer of the substrate lattice. For a submonolayer coverage of two-dimensional islands, this would mean a relaxation of the substrate layer beneath the deposited islands and near their edges. If the deposited islands are placed on large substrate terraces, the two-dimensionally extended substrate layer around the islands can only relax slightly to stresses. However, if the deposited islands occur near the upper edge of substrate steps, the topmost substrate layer can relax more easily because of the broken symmetry along the step.

In our special case of submonolayer Fe film growth on Cu(111), there is a lattice mismatch between bcc Fe and fcc Cu, which are the thermodynamically stable lattices of both metals at 300 K. However, it is well known [1,11] that Fe deposited onto Cu(111) at room temperature is forced to grow initially in a pseudomorphic way, probably assuming the structure of a slightly distorted fcc phase with a misfit of -0.7%. LEED intensity analyses [21] revealed that this strained pseudomorphic growth proceeds up to a thickness of about 4–5 layer equivalents before a phase transformation to bcc Fe(110) layers in the Kurdjumov–Sachs orientation occurs. However, from our STM investigation, it follows that fcc Fe does not grow layer by layer from the beginning of deposition. Only at the upper sides of Cu steps are Fe islands of 1 ML thickness formed, whereas on the terraces, bilayer Fe islands are seen (Figs. 2 and 3). These different metastable states of fcc Fe on Cu may be due to the interaction of strained Fe islands and the Cu substrate. In the vicinity of Cu steps, the uppermost Cu layer can relax the tensile stress of the fcc Fe deposit, thus possibly stabilizing monolayer nucleation and growth. On the other hand, the more rigid topmost Cu layer of extended terraces forces the Fe islands to grow as bilayers. Moreover, fcc–bcc transformation starts locally as early as the third monolayer of Fe on top of the bilayer islands [17].

The relaxation of the Cu lattice near the Cu steps (due to the tensile stress of Fe islands) results

not only in the locally different growth modes mentioned above, but also induces the formation of Cu holes. In general, lateral stress in the surface layer may change the activation energy for the surface diffusion of adatoms, or the activation energy for edge diffusion along steps. Since the uppermost Cu layer relaxes more easily near steps, we expect the most pronounced changes in the Cu diffusion processes near steps where monolayer Fe islands exert tensile stress.

We now outline our strain-driven mechanisms of hole formation in detail. As a first prerequisite to the model, we note that on a clean Cu(111) surface at 300 K, the mobility of adatoms and kinks along ⟨110⟩ atomic steps is high, causing frizzy steps in the STM images [15,16]. On a clean Cu(111) vicinal surface, this diffusion process causes local fluctuations in the step distances, but no bulging (see Fig. 1). Two conditions have to be fulfilled for the erosion process to start and proceed. First, the movement of the underlying Cu step has to be stopped locally by the presence of immobile Fe islands at the step edges. Second, there must be a driving force to induce erosion between adjacent Fe islands, including the edge energy of the increasing step length of the new hole. We presume the tensile stress around the Fe islands to be the driving force in the initiation and growth of holes.

The relaxation of the Cu lattice near the Cu edges owing to the tensile stress of the Fe islands slightly diminishes the binding and activation energies for Cu edge diffusion. Therefore, Cu edge diffusion and the emission of Cu atoms on the terraces are enhanced, enabling a net mass transfer from the eroded parts of the Cu steps between the immobile Fe islands to the lower Cu terraces. This erosion is the starting point of hole formation at steps (Fig. 1). Once a hole is formed, it proceeds to grow along step edges (Fig. 2) because the driving force acts preferentially along the chain of Fe islands, thus forming oblong-shaped holes. Furthermore, the very slow hole growth leads to the hexagonal shape of the holes, which tend to assume the equilibrium shape of two-dimensional negative crystals. For holes with openings to the descending terrace (Fig. 2), only the close-packed ⟨110⟩ directions of the holes indicate the near-equilibrium stage, whereas the oblong shape is due to the preferential strain effect along the Fe chains. Only the isolated Cu holes on the terraces (at D and below C in Fig. 5a) assume their equilibrium shape, with {100} and {111} microfacets of equal lengths facing each other. Isolated holes (Fig. 5a, D) start a Brownian movement over the terrace as a function of their size by thermally activated processes of adatom edge diffusion or by adatom emission into the holes, as discussed in Ref. [18]. The Cu atoms leaving the holes are spread along Cu steps, or diffuse across the terraces to the next descending steps, or are trapped at Fe islands (Figs. 3 and 4). This tensile-strain driven mechanism proceeds with increasing Fe coverage until the openings of the holes are sealed by the coalescence of the chains of Fe islands forming continuous wires, as shown in Figs. 7 and 8. Then, the hole formation process at Cu steps as discussed so far stops.

However, another hole formation process starts near the Fe wires at the upper step edges, resulting in large extended holes on the Cu terraces (Fig. 8). As a consequent extension of our first strain-driven mechanism, we assume that with increasing width (0.2–0.5 of the mean step distance) and height (2–3 ML) of the Fe wires, the strain fields along the wires increase to such an extent that they enable the formation of Cu surface vacancies and holes by the step-upward diffusion of Cu. This hole formation process and the step-upward diffusion results partially in 1 ML Cu patches covering the Fe wires. This can be proved by spectroscopic STM imaging [8]. Surprisingly, the growth rate of holes in the latter case is of the same order of magnitude as that at steps, as discussed above.

From these considerations, the suppression of hole formation can be explained quite easily. Lowering the deposition temperature from 300 K to 250–273 K is enough to freeze out both hole formation processes effectively during a deposition time of some minutes at most. The sealing of Cu steps and Fe wires by depositing 0.2 ML Au to avoid repeated hole formation after warming up to 300 K is based on the following consideration. Metals with surface energies close to that of Ag ($1.25\ J\ m^{-2}$) or Au ($1.55\ J\ m^{-2}$) and lower than that of Cu ($1.85\ J\ m^{-2}$) should wet the Cu steps,

which has been confirmed experimetally (Fig. 6). Furthermore, relative to Cu, both Ag and Au have larger lattice constants, or a positive misfit of about 13%. They therefore exert compressive strain, thus eliminating the tensile-strain sources for both hole-formation mechanisms.

The strain-driven hole formation discussed for the system Fe/Cu(111) has also been proved to be applicable to the system Co/Cu(111). Hence, hole formation is suppressed in the same way.

5. Conclusions

STM was used to study the formation and growth of 1 ML deep holes on a Cu vicinal surface after the deposition of Fe in the range of submonolayer coverage at 300 K. A new strain-driven mechanism is proposed, explaining the initiation of the erosion of step regions between the immobile Fe islands at the upper step edges as the first stage of hole formation. The driving force results from a tensile strain field between and around the Fe islands at the Cu step edges, which causes the uppermost Cu layer to relax near the steps, thus inducing a net diffusion flux out of the holes. The growth of the hexagonal-shaped Cu holes preferrentially along the chains of Fe islands at the steps and the spreading to large extended holes between the steps are also strain-driven, and proceed as long as the holes have openings. The Cu material removed from the holes is distributed either along the Cu steps owing to edge diffusion, or it diffuses to the next descending Cu steps via the Cu terraces, or is trapped at Fe islands. This hole formation process stops with increasing Fe coverage on sealing the openings at the steps. For Fe coverages high enough to form continuous wires and thus to seal all possible openings, the increasing strain fields along and between the Fe wires open a new step-upwards diffusion path for another hole-formation and growth process.

The formation of holes can be suppressed completely by depositing Fe at lower temperatures and sealing the Cu steps or Fe wires by a step-bottom decoration with Ag or Au. At low temperatures, the diffusion processes of Cu kinks and adatoms are frozen out. The wetting of the Cu steps or Fe wires by Ag or Au exerts compressive strain, thus annihilating the driving force for further hole formation when warming to 300 K.

This investigation demonstrates the complexity of phenomena in epitaxial systems, in particular the subtle balance between diffusion processes and experimental parameters such as temperature, coverage and stress in heterogeneous systems. As the new model does not imply any alloying between Fe and Cu, there may be no deterioration of the magnetic properties of quasi-one-dimensional magnetic Fe wires. This, however, is still under study.

Acknowledgements

The authors are indebted to the Thyssen Stiftung for their financial support of the multi-chamber facility. Special thanks are due to Mrs. F. Pabisch and Mr. G. Kroder for technical assistance during the experiments.

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