

## Segregation-mediated capping of Volmer-Weber Cu islands grown onto Ag(111)

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The growth of Cu on an Ag(111) surface is studied using scanning tunneling microscopy at room temperature and for low Cu coverage ranging from 0.02 to 1.5 monolayers. Three-dimensional islands are found to grow at the Ag surface steps. During this Volmer-Weber growth, the erosion of steps and the formation of vacancy domains inside the terraces indicate that a large redistribution of Ag atoms takes place. Moreover, STM images from the top of islands reveal a  $(9 \times 9)$  reconstruction which is well known to occur in the reverse case, where one Ag monolayer is deposited on Cu(111). These findings combined with molecular dynamics simulations allow us to conclude that the Cu islands are capped, from the very beginning of the growth, by one monolayer of Ag atoms diffusing from the eroded regions.

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### I. INTRODUCTION

For several decades, thin heteroepitaxial metal on metal growth has received considerable attention from both applied and fundamental science points of view. It is well known that during growth there is a complex competition between the equilibrium parameters of the couple deposit/substrate (e.g., interface and surface energy, enthalpy of mixing, mismatch, etc.) and the growth kinetics (e.g., deposition rate, deposition energy, mobility via growth temperature, etc.). From Bauer's pioneering works based on equilibrium arguments<sup>1,2</sup> to more recent kinetic treatments<sup>3,4</sup> most of the growth modes can be well captured. However, some systems still exhibit surprising and unexpected behaviors. Let us recall, for example, the surface confined alloying that occurs for bulk immiscible systems,<sup>5</sup> or more surprisingly the spontaneous substrate surface etching (with noncorrosive deposit) during metal deposition.<sup>6-9</sup>

The Ag-Cu system can be considered as a model one to study the growth of an immiscible and largely strained system. Indeed, Ag and Cu present a 13% mismatch and a large positive enthalpy of mixing.<sup>10</sup> Moreover, due to the large surface energy difference between Ag and Cu [ $1.24 \text{ J/m}^2$  and  $1.8 \text{ J/m}^2$ , respectively, for Ag and Cu (Ref. 11)] this system is also a model one, such as Ni-Cu, Fe-Cu, Fe-Ag, Rh-Ag, or Co-Cu,<sup>12</sup> to study segregation effects. The heteroepitaxial growth, in UHV environment, of Ag on Cu(111) oriented surface is well documented. In the range of 0–2 monolayers (ML), a layer-by-layer growth is observed by scanning tunneling microscopy (STM).<sup>13,14</sup> Large Ag islands of 1 ML height characterize the morphology at submonolayer coverage. Surface diffraction analysis<sup>2,15</sup> and STM experiments<sup>16,17</sup> revealed a characteristic  $(9 \times 9)$  superstructure of the Ag surface. Two competing atomic structures are reported to explain this  $(9 \times 9)$  superstructure: the “Moiré” one observed at 150 K, and the “triangular” one observed at room temperature (RT). The Moiré structure involves a con-

tinuous matching between deposit and substrate, whereas the triangular involves vacancies in the first Cu layer leading to fcc/hcp stacking fault limited by triangular loop of dislocation.<sup>17</sup> Not any mixing, nor surface alloying, even at low coverage, is reported in Ag/Cu(111) at RT.

The Cu/Ag(111) growth has not been extensively studied as the Ag/Cu(111) one. It was already reported that Cu films are (111) oriented on Ag(111) with  $\text{Cu}\langle 110 \rangle // \text{Ag}\langle 110 \rangle$ .<sup>18</sup> Concerning the growth, both the Stranski-Krastanov mode<sup>19,20</sup> and the Volmer-Weber mode<sup>21</sup> have been reported at RT for two or three deposited Cu monolayers on Ag(111). Therefore, the growth mode in this early stage of deposition is still under debate. In this article, we study the growth of Cu on Ag(111) from submonolayer up to 2 ML at room temperature by using scanning tunneling microscopy. This is, to our knowledge, the first investigation in the direct space that focuses on this growth. In Sec. II, experimental conditions are briefly reported. In Sec. III, we elucidate the growth mode. We show that the Cu/Ag(111) growth, which belongs formerly to the Volmer-Weber scheme, turns out to be highly complex due to the occurrence of a capping process of Cu islands by silver. To provide an atomic picture of this growth mode, we also present in Sec. IV molecular dynamics simulation results on this system. A conclusion is given in Sec. V.

### II. EXPERIMENT

The experiments were conducted in a multichamber vacuum system with a base pressure in the  $10^{-10}$  Torr range. LEED, XPS, and STM observations can be performed in the characterization chamber. Cu depositions were performed in the preparation chamber at RT. Cu is evaporated from resistively heated crucible. The evaporation rates were around 1 ML in 240 s for all the experiments presented here. The calibration of the evaporator was done by a combination of XPS and STM observations. We estimate its absolute accuracy at around 20%. All the coverages indicated were obtained from

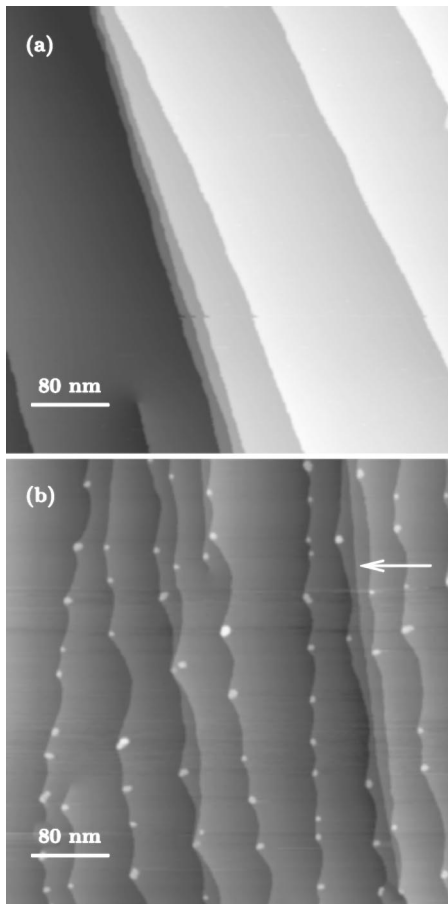


FIG. 1. (a) STM image, acquired at room temperature, of a clean Ag(111) surface after preparation cycles. (b) STM image of 0.02 ML Cu on Ag(111) grown at RT. This image illustrates the large step destabilization found even at low coverage. Large baylike steps link the 3D islands.

the evaporation time by using this calibration rule.

The Ag substrate is a monocrystal (111) oriented, mechanically and chemically polished. Cleaning of the substrate consists of many cycles of Ar-ion bombardment (2.5 KeV ion acceleration, and  $10^{-6}$  Torr Ar pressure) at RT during 15 min, before annealing at 550 K. Cycles were repeated until a sharp  $(1 \times 1)$  LEED diffraction pattern with a low background is achieved, and no contamination could be detected neither by XPS nor on large STM images. Terraces of 80 nm width could be found easily on STM observations.

STM experiments were always performed at RT, on an as-deposited sample. The time interval between the end of deposition and the first image acquisition is around 15 min. No evolution of the surface morphology was observed during the STM experiments. Typical experimental conditions for obtaining images were a tunneling current ranging from 0.1 to 1 nA, a voltage ranging from  $\pm 0.1$  to  $\pm 1$  V, and a scanning speed around 1000 nm/s, depending on the morphology of the surface.

### III. STM RESULTS

Figure 1(a) shows the typical surface of Ag(111) after

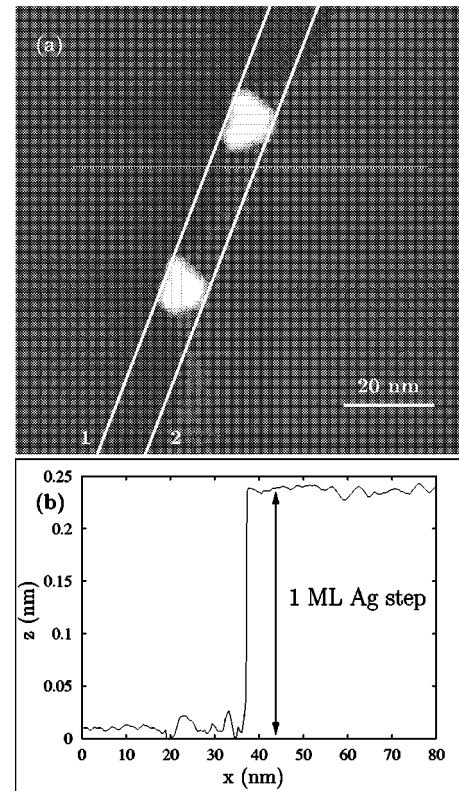


FIG. 2. (a) High-resolution image of the 0.02 ML Cu deposition shows details on the relative position between island and step. The thick white lines (labeled 1 and 2) bound the initial Ag step position before deposition. (b) Height profile along the horizontal white line.

preparation. Large terraces separated by monoatomic steps are evidenced. Some merging dislocations can also be observed. Due to local misorientation, steps are not always along a particular direction. Nevertheless, steps are straight on few hundred nanometers length, and no damage (such as hole or huge roughening) can be observed on the clean Ag surface. The Fig. 1(b) shows the surface for a low coverage of 0.02 ML, it reveals that islands are 0.4–0.7 nm height. Even at this low coverage, island heights are larger than one monoatomic Cu(111) step (i.e., 0.209 nm). Density of islands is around  $3.8 \text{ islands}/10^4 \text{ nm}^2$ . As shown in Fig. 2(a), islands present facets parallel to the  $\langle 111 \rangle$  directions. All islands, even on terraces larger than 130 nm (not shown here), are located at step edges: the nucleation is clearly step induced. Density of islands along a step is, on average, around 0.02 islands/nm but seems to be dependent on the adjacent terrace size. Another striking result is the important change of morphology of the step edges. These steps are no longer straight [compare Figs. 1(a) and 1(b)], but adopt a bow shape between two consecutive islands. This morphology is tightly related to the Cu deposition and can not be due to the preparation of the Ag substrate. Very rare steps do not present attached Cu island [see the marked step in Fig. 1(b) separating two very short terraces]. It is noteworthy that such a step without Cu island stays straight.

In addition, a cross-section measurement in Fig. 2(b) shows that even at the vicinity of an island, the step height is 0.24 nm that is the Ag monoatomic step height. Therefore,

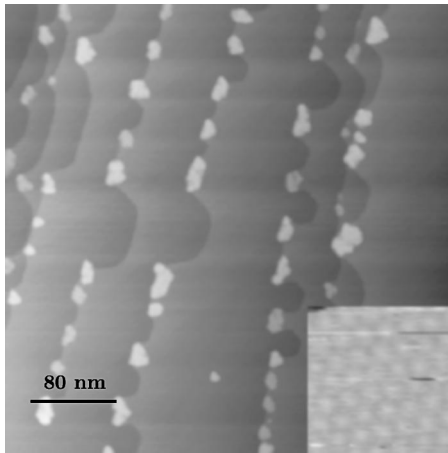


FIG. 3. STM image of 0.3 ML Cu on Ag (111) grown at RT. The increased etching results now in large faceted vacancy cluster developed along the steps. In the inset ( $12 \times 12 \text{ nm}^2$ ), a high-resolution image on top of an island shows a  $(9 \times 9)$  superstructure pattern.

this step destabilization between two consecutive islands appears as a consequence of the rearrangement of Ag atoms along steps. However, this important redistribution of matter at the Ag steps makes the determination of the initial step position difficult. From STM images one can simply delineate two extreme positions for the initial Ag step position [see Fig. 2(a)]. Depending on the line considered, one could envisage either an erosion process of the step between the two islands (line 1) or a complex redistribution of the matter at the step and around the islands (line 2).

Figure 3 presents the surface morphology for a 0.3 ML Cu deposit. Density of islands is still around  $3.8 \text{ islands}/10^4 \text{ nm}^2$ . Though few coalescence events can be observed, increasing the coverage from 0.02 to 0.3 ML does not modify significantly the nucleation density. Thus the initial nuclei, located at step edges, have simply grown. We note that islands exhibit elongated shape consistent with a preferential growth along the step. At 0.3 ML Cu islands are 0.5–1 nm height, 10–16 nm width, and 13–32 nm length. Islands, at least the largest ones, are less faceted than those observed at 0.02 ML. By comparing Figs. 1(b) and 3, it is worth noticing that the destabilization of the steps has largely increased. Indeed, large erosion is observed on some step parts leading to semicircular opened islands of vacancies. These large 1 ML vacancy islands adopt equilibrium shapes with facets. A reliable measurement of the eroded area is impossible, but the quantity of displaced Ag atoms is clearly related to the Cu coverage value. As island size increases, so does the step erosion. One can point out, from Figs. 1(b) and 3, that islands never appear inside eroded regions. According to Klaua *et al.*,<sup>9</sup> this absence of island in bowed step is understood when erosion takes place after nucleation and growth of islands. As shown in the inset of Fig. 3, the structure of the island top has been resolved by STM. An hexagonal superstructure with a  $2.4 \pm 0.1 \text{ nm}$  cell size is evidenced.

Figure 4 has been image processed to make the steps more visible. It shows the morphology of the surface after a 1.5 ML Cu deposition. Density of islands has decreased to

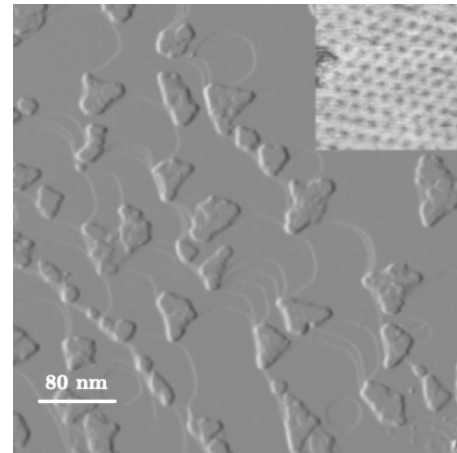


FIG. 4. STM filtered image of 1.5 ML Cu on Ag(111) grown at RT. By increasing the Cu coverage the step etching is now so important that the vacancy bay extend over the entire upper initial terrace. Some vacancy cluster can be observed. In the inset ( $18 \times 18 \text{ nm}^2$ ), a high-resolution image on top of an island reveals again a  $(9 \times 9)$  superstructure pattern.

$2.3 \text{ islands}/10^4 \text{ nm}^2$ . Islands are 20–70 nm width and about 1.5 nm height, they do not adopt regular shape. Moreover, the terrace erosion is now so pronounced that some vacancy islands extend over the entire terrace, which sometimes gives rise to complex multilevel step profile. In addition, it is interesting to note that on some terraces, this large erosion process forms monoatomic hexagonal vacancy islands. Once more, Fig. 4 shows that the step erosion increases with the Cu coverage. At this coverage, high-resolution images could again be achieved on the top island (see the inset in Fig. 4). Both superstructures observed in Figs. 3 and 4 are compatible with a  $(9 \times 9)$  pattern on Cu(111). Generally, in a STM image, it is difficult to distinguish the chemical nature of the imaged atoms. But let us just recall for the moment that such superstructures are very similar to the well documented superstructures obtained when one silver monolayer is deposited onto Cu(111). This point will be clarified below by taking into account the results of simulation in the next section. We will demonstrate that an Ag capping layer reconstruct the top most surface of Cu islands.

#### IV. SIMULATIONS AND DISCUSSION

Several noticeable results can be directly drawn from STM data: (i) the nucleation proceeds along initial Ag step edges. (ii) A 3D-growth belonging to the Volmer-Weber mode is evidenced from the very beginning of the growth (even at low coverage  $< 0.02 \text{ ML}$ ). (iii) The initial straight Ag step adopts a bow shape in between two Cu clusters, with a curvature that increases with the cluster size. (iv) STM atomic resolution reveals a  $9 \times 9$  reconstruction on top of Cu island which looks like the one observed for 1 ML Ag/Cu(111). These last two observations strongly support a segregation process of Ag atoms and the capping of Cu islands. Let us first briefly discuss the first two points. The heterogeneous nucleation along the steps implies a fast dif-

fusion of Cu adatoms on Ag(111) surface, then along steps. Copper adatoms attach and nucleate at steps where they can find highest reactive sites. This reactivity may be also enhanced by stress as reported in Ref. 9 The observed 3D growth is consistent with the Bauer criterion, since Cu deposited atoms present a surface energy lower than Ag substrate atoms. However, step edges, large misfit between the two elements and the possible segregation of Ag atoms on top of the Cu islands are also supposed to influence the 3D growth regime and island shapes. These effects are also related to the two last points (iii), (iv) we discuss now.

The destabilization of substrate steps followed (or not) by the formation of vacancy islands has been observed in different metal on metal systems. In the case of Fe/Cu(111),<sup>9</sup> the hole formation is not correlated to the Fe coverage and seems to be related to the stress relaxation. In the case of Fe/Cu(111) (Ref. 7) it is shown that the stress is responsible of the Cu enhanced desorption from the steps to a 2D adatoms gas giving rise to large reorganization of the surface. In the case of Ir/Cu(111),<sup>22</sup> intermixing and subsurface alloying induce step etching. For Co/Cu(111) (Refs. 23 and 24) and Al/Pt(111) (Ref. 25) surface alloying produces vacancies that condense to form hexagonal holes near steps. In Rh/Ag(100) (Refs. 6 and 8) the etching of steps provides the amount of Ag necessary to encapsulate Rh atoms.

In the case under investigation, we clearly show that the Ag step destabilization and the migration of Ag atoms are correlated to the Cu coverage value. In addition, the eroded zones do not contain any islands. These observations tend to assume that the island formation precedes the Ag step destabilization. We have already mentioned that the  $(9 \times 9)$  superstructure obtained on the islands is analogous to the 1 ML Ag/Cu(111) case. In addition, according to some recent Monte Carlo simulations performed on the dilute Cu(Ag)(111) system,<sup>26</sup> such superstructures should appear by an Ag surface segregation process. Therefore, it is reasonable to assert that Ag atoms cap, at least on the top, the Cu islands. Due to the difficulty to determine exactly the quantity of Ag atoms displaced, we cannot, however, confirm the complete absence of exchange between Ag and Cu atoms at step edge or alloying inside the islands.

In summary, our STM results suggest the following mechanism for the Cu/Ag(111) growth mode at low coverage and RT: pure Cu islands nucleate at step edge and pin it locally as observed in Cu/Ag(100).<sup>27</sup> Then, Ag atoms from the surrounding step edges diffuse along the step to encapsulate the Cu islands. We conjecture that the main driving force that controls this stage is the gain in surface energy. Indeed, a simple calculation allows us to compare the line energy cost to create curved Ag step and the surface energy gain to cover Cu(111) island by Ag(111). The energy cost is overestimated by taking a circular Ag vacancy cluster of radius  $R$  [this energy cost is correctly estimated from the line energy of  $\langle 110 \rangle$  Ag steps on (111) surface<sup>28</sup> ( $1.38 \times 10^{-10}$  J/m) since they are those steps which are created by the erosion process], while the energy gain for capping an equal Cu(111) circular surface of radius  $R$  by Ag(111) is obtained from surface energy difference. One find that encapsulation is favored as soon as the radius  $R$  exceeds a few

Å. Thus, based on this simple calculation, the surface energy decrease could generate an efficient driving force even for the low Cu coverage cases considered in this work. In addition, Ag atom migration from step towards Cu islands should be kinetically reachable since, even at RT, it has been already shown that the Ag mobility is significant along step edges.<sup>27,29</sup> Thus, based on these qualitative arguments the capping of Cu islands by Ag atoms should occur at the expense of the Ag step etching. Of course, several local effects have been neglected in this simple global approach. Island mobility, shape, and composition should affect the encapsulation mechanism. The effect of stress on the Ag mobility<sup>30,31</sup> and on a possible surface alloying<sup>32</sup> may also play an important role. One can wonder what is the precise atomic Ag rearrangement inside and around the islands.

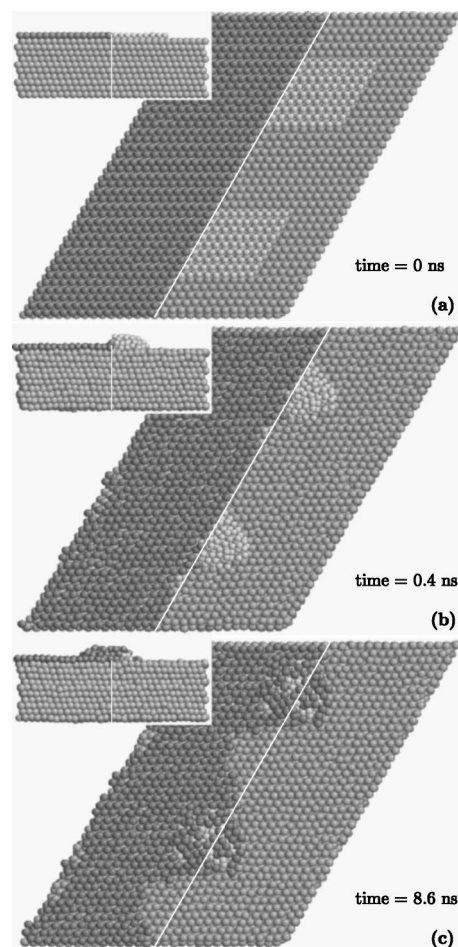


FIG. 5. Sequence of snapshots taken from the molecular dynamic simulations performed at  $T=800$  K using the SMA potential: (a) an initial flat 81 Cu atom cluster (white spheres) is built at the vicinity of an Ag step (dark spheres) on a (111) Ag surface slab (grey spheres), (b) after 0.4 ns, Cu atoms form a 3 Cu ML height cluster attached to the Ag step, (c) after 8.6 ns, the cluster moves inside the Ag step and is made of 2 pure Cu ML covered by 1 pure Ag ML. The Ag encapsulation takes place with the destabilization of the Ag step adopting a baylike shape. The insets show a view along the initial Ag step represented by a white line. Notice that each snapshot contains two simulation boxes to emphasize this bay formation.

In order to provide a more realistic atomic picture of this process, we performed molecular dynamics (MD) simulations using an Andersen thermostat (see, for instance, Ref. 33). The second moment approximation (SMA) potential is used to describe atom interactions with parameters from Ref. 34. The parameters were adjusted to reproduce interatomic distances, cohesive energies, elastic constants, and the strong tendency to phase separate in the Cu-Ag system. Although exact surface energies were underestimated within the SMA potential, the difference in surface energies of the two elements Cu and Ag is correctly yielded.

To study the morphology of Cu clusters at the vicinity of Ag steps and their possible encapsulation by Ag, one considers the initial configuration shown in Fig. 5(a). A slab made of ten (111) Ag layers of 600 atoms with periodic conditions in the  $\langle 111 \rangle$  directions is built in order to mimic the fcc Ag substrate with two surfaces. On the upper side of the slab, one wants to simulate two Ag terraces separated by one [110] step. In practice we cover one half of the surface with an Ag(111) strip and due to the periodic conditions of the simulation box these additional Ag atoms represent an Ag terrace bounded by two Ag[110] steps. Finally, on one side of the ascending Ag step, we build an arbitrary flat island of 81 Cu atoms on the fcc surface sites. The total amount of atoms considered in the simulation is 6381 and, to observe on a MD time scale (here in nanoseconds) a significant mass transport, we consider in the simulation a temperature much higher than the experimental one (i.e.,  $T=800$  K). The cell dilatation due to the temperature is taken into account in the initial slab construction. Figure 5(b) shows the very beginning of the kinetics at  $t=0.4$  ns. One can observe that most of the Cu atoms have moved to form a pure 3D island while the straight Ag step is almost unchanged. Rare isolated Cu atoms are found to be incorporated in the Ag step. A view along the Ag step shows that the 3D island remains attached to the Ag step and presents a 3 Cu layers height. More surprising is the configuration reached after 8.6 ns. Indeed, one can observe in Fig. 5(c) a complete change of both the cluster composition and the step shape. During this stage, the Cu cluster moves inside the Ag step. Indeed as shown in the Fig. 5(c), the center mass of the cluster is located on the initial Ag step position. This result underlines the difficulty to locate experimentally the initial step position [see Fig. 2(a)]. Concerning the cluster composition, we note that a capping Ag atom layer took the place of the topmost Cu atom layer. The Cu cluster is now made of two almost pure Cu layers covered by an almost pure Ag layer. Very few isolated Cu atoms are found under the cluster in the former Ag surface plane, or around the cluster, within the Ag terrace. Let us add that most of the Ag atoms having diffused around or on the cluster originates from Ag step edges. This process induces a drastic change of the step shape. Indeed when the Cu cluster migrates towards the upper terrace, it necessarily induces an

Ag displacement from that terrace. One finds that the number of Ag atoms involved in this process is insufficient to fully encapsulate the Cu cluster. Additional Ag atoms have to diffuse along the step to complete the Ag capping layer. This long distance diffusion along a step in between two clusters (here, in the simulation in between the cluster and its periodic image) leads to the bowing of the Ag steps [see Fig. 5(c)]. In addition, let us mention that we have also considered the initial configuration where the flat Cu island is located at the descending step. The resulting simulations (not shown here) lead to an atomic rearrangement very similar to the one shown in Fig. 5(c). In summary, the results of MD simulations confirm the STM observations. Silver atoms migrate from upper terraces and steps to cap the Cu islands under the segregation driving force.

## V. CONCLUSION

Using scanning tunneling microscopy, we have studied the early stage of the Cu growth on an Ag(111) substrate at room temperature. First, we unambiguously show that the growth mode is a Volmer-Weber one. This latter proceeds by the nearly exclusive nucleation of 3D Cu islands at the step edges of the Ag(111) surface. Moreover, this 3D growth takes place with a surprising large Ag step etching, forming large bays between two consecutive islands. Such a destabilization of step morphology is due to the tendency of the Ag atoms to segregate on top of 3D Cu clusters which are finally capped. This conclusion could be drawn from both concordant STM data and MD simulations.

(i) A  $(9 \times 9)$  reconstruction very similar to the well known one reported when 1ML Ag is deposited onto Cu(111) is evidenced by STM on top of Cu islands grown onto Ag(111). STM also reveals the important erosion of steps that become curved.

(ii) Molecular dynamic simulations confirm the important moving of atoms leaving steps that become curved in between islands, and the diffusion of Ag atoms from step towards Cu islands they finally cap.

When Cu atoms are deposited onto Ag(111), Cu islands are created at steps, following a formerly Volmer-Weber growth mode. However, the growth mode appears more complicated than expected from the simple Volmer-Weber scheme since, from the very beginning of the growth, the segregation effects lead to the capping of Cu islands by an Ag monolayer.

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