PHYSICAL REVIEW B **76**, 115417 (2007)

Upward self-diffusion of adatoms and small clusters on facets of fcc metal (110) surfaces

Haili Yang,[1] Qiang Sun,[1] Zhenyu Zhang,[2,3] and Yu Jia[1,2]
[1]*School of Physics and Engineering, Zhengzhou University, Zhengzhou 450001, China*
[2]*Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6062, USA*
[3]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*

(Revised manuscript received 7 April 2007; revised manuscript received 25 July 2007; published 13 September 2007)

We study upward self-diffusion of adatoms and small clusters on faceted huts formed in fcc metal (110) homoepitaxy using molecular dynamics simulations with interatomic potentials described by the embedded-atom method. Our results show that both individual adatoms and small clusters on the (111)-sloped and (100)-sloped facets of the huts on Al and Cu(110) can readily diffuse upward and cross the convex edges of the huts, but with different atomistic mechanisms. An adatom crosses the convex edges via a simple concerted exchange or indirect place exchange mechanism. In contrast, the upward diffusion and convex-edge crossing of small clusters is realized by their dissociation at or near the edges of the hut after one or two atoms belonging to the cluster are incorporated into the edges. The present simulation studies reveal that there truly exists efficient upward mass transport on faceted islands in fcc metal (110) homoepitaxy, and such upward diffusion processes are expected to play an important role in defining the kinetic faceting instability in these growth systems.

DOI: 10.1103/PhysRevB.76.115417 PACS number(s): 66.30.Fq, 68.35.Bs, 68.35.Fx, 68.35.Ja

I. INTRODUCTION

It has been well accepted that the selection of a specific growth mode in a given system is often the outcome of the interplay between growth kinetics, characterized by a set of atomic rate processes, and thermodynamics, driven by the system's overall tendency toward lower free energy configurations.[1] Since the regulation can be realized through the movements or the diffusion behaviors of adatoms and small clusters, the first step toward a detailed understanding of surface morphology during and after growth is to identify all the important atomic rate processes. Once the diffusion behaviors of all the elemental entities are known, the evolution of the surface morphology during growth may be predicted and a desirable growth mode is likely to be selected via manipulation of the growth kinetics. On the other hand, determining the key currents and facet and step energies is also important because it determines the evolution and allows one to check whether all atomistic processes of importance have been included.

Up to now, extensive theoretical and experimental studies of the diffusion of adatoms and small clusters in homoepitaxial growth have been carried out for various systems, such as on the low Miller index surfaces of Cu, Al, and Pt (Refs. 2–16) and at stepped surfaces of Al(111),[4] Cu(001),[10] Ir(111),[11] and Ag(111).[12] In the latter cases, the focus had been primarily on downward diffusion at the edge of monatomic steps.[8,15,17–19] Here, a descending adatom will encounter an additional potential energy barrier [Ehrlich-Schwoebel (ES) barrier[20,21]] at the step edge. If the ES barrier effect is sufficiently weak such that the adatoms can easily climb down the steps, two-dimensional growth of smooth films can be achieved. In the opposite regime, where the ES barrier effect is strong, three-dimensional morphology will appear, characterized by the formation of surface mounds and rough films.[1,22–24]

Very recently, an intriguing observation of faceting instability was reported by Buatier de Mongeot *et al.* in experimental studies of Al(110) homoepitaxy.[25] They found that, under proper growth conditions, regular pyramidal islands bounded by four extended facets were formed after deposition of ~10 ML (monolayer) of aluminum or higher. These hut-shaped islands are ten times as tall as the average thickness of the deposited film and have precise slope selections. Detailed analysis of the huts along the two principal crystallographic directions of ⟨100⟩ and ⟨110⟩ reveals that the major and minor facets are terminated by the {111} and {100} planes, respectively. The formation of the huts could not be attributed purely to insufficient downward adatom diffusion within the framework of the ES barrier effect; instead, their unusual heights demand the existence of massive atom transport from the terraces onto the growing huts. To resolve this puzzling observation, extensive first-principles calculations of activation energies have been carried out within density functional theory (DFT) for adatom diffusion on and around monatomic and multilayer steps on Al, Pb, Cu, and Ag (110).[25–27] The DFT results showed that there exist efficient kinetic pathways for true upward adatom diffusion, and simplified one-dimensional kinetic Monte Carlo simulations using these atomic rate processes as inputs illustrated the faceting instability for the formation of the huts.[25–27]

The DFT calculations were performed for adatom diffusion using relatively small supercell sizes and at zero temperature. One intriguing question that we examine is whether small clusters formed on the faceted islands could also diffuse upward, cross the convex edges, and add themselves to the top of the huts. If small clusters could not diffuse away or dissociate fast enough, their formation on the facets would roughen the facets, thereby eliminating the possibility of precise slope selection in the formation of the faceted huts. For studying the mobility of small clusters, it is more desirable to carry out direct molecular dynamics (MD) simulations at finite temperatures, as such approaches are better suited to uncover complex atomic processes of concerted nature.

This is the objective of the present study: We carry out extensive MD simulations of the diffusion of both adatoms and small clusters on the (111)-sloped and (100)-sloped facets of huts formed on Al and Cu(110) surfaces, at various temperatures, and with interatomic potentials described by the embedded-atom method (EAM).[28–31] The possible importance of lattice expansion due to the elevation of temperature is also considered. Our results show that it is favorable for both adatoms and clusters to diffuse upward and cross the convex edges of the facets, but with different atomistic mechanisms. An adatom crosses the convex edge via a simple concerted exchange or indirect place exchange mechanism. In contrast, for small clusters, the upward diffusion and convex-edge crossing is realized by a combination of cluster dissociation at the edge and concerted exchange between the atoms belonging to the cluster and the edge atoms of the hut. Our MD simulations reveal that there truly exists efficient upward mass transport on faceted huts in fcc metal (110) homoepitaxy, and such upward diffusion processes of both adatoms and small clusters are expected to play an important role in defining the kinetic faceting instability in these systems.

The paper is organized as follows. In Sec. II, we briefly describe the EAM and the technical aspects of the MD simulations. In Sec. III, we present the simulation results for upward self-diffusion of individual adatoms on the (111)-sloped and (100)-sloped facets of a hut on an Al(110) surface. The results for small clusters (dimer, trimer, and tetramer) diffusing on the (111) facet of a hut on Al(110) are presented in Sec. IV. Section V contains the results for Cu adatom or cluster diffusion on the Cu(111)-sloped and Cu(100)-sloped facets, aimed to explore the general aspect of the kinetic processes. Discussions and conclusions are presented in Sec. VI.

II. MODEL SYSTEMS AND COMPUTATIONAL DETAILS

The embedded-atom method is a semiempirical simulation method with input parameters drawn from experimental values.[28–31] The basic idea of the EAM is that the total electron density in a metal can be approximated by the superposition of the electron densities of the individual atoms within the metal, and the energy of an embedded atom is determined jointly by the total electron density at the position where the atom resides plus the sum of pairwise potentials characterizing the core-core repulsion of atomic nuclei within a given cutoff distance. The energy of the ith embedded atom is then written as

$$E_i = \frac{1}{2}\sum_{j \neq i} \Phi(r_{ij}) + U(\rho_i), \tag{1}$$

where the first term represents the pairwise repulsive potential, r_{ij} is the distance between atom i and atom j, and the second term is the energy required to embed atom i into the background electron density. The electron density ρ_i is also taken to have a pairwise form

$$\rho_i = \sum_{j \neq i} f(r_{ij}), \tag{2}$$

where f is the electron density from each neighboring atom of the embedded atom i.

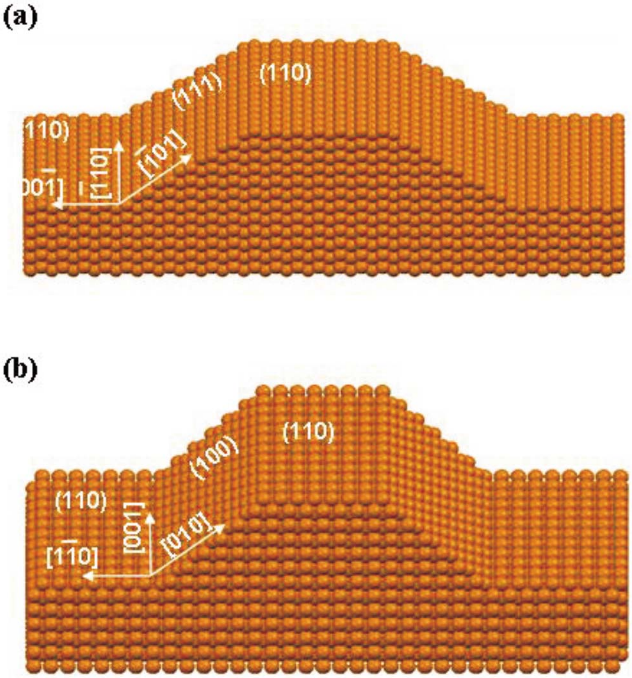

FIG. 1. (Color online) Simulation models of an Al hut island on a (110) surface, with different sloped facets: (a) (111)-sloped facet and (b) (100)-sloped facet.

In the past, the EAM potential has been shown to give reasonably accurate descriptions of the bulk and surface properties of metal and alloys,[32,33] such as bulk stress, chemisorption at surface, surface diffusion, and surface vibration.[32–38] In our present study, we use two model systems to study the upward diffusion processes, corresponding to adatoms and clusters ascending at the step edges along both the $\langle 110 \rangle$ and $\langle 100 \rangle$ directions on the (100)-sloped and (111)-sloped facets of a hut on the Al(110) and Cu(110) surfaces, respectively (Fig. 1). Models with a 12-layer hut on a 12-layer (110) substrate are used in our calculations. Periodic boundary conditions are utilized along both the x $[00-1]$ (or $[-110]$) and y $[-110]$ (or $[001]$) directions for a (111)-sloped [or (100)] facet. In studying adatom upward diffusion on the (111)-sloped facet, the size of the substrate is $10\sqrt{2}a_0 \times 28a_0$, while that of the (111)-sloped facet is $10\sqrt{2}a_0 \times 3\sqrt{6}a_0$, and the (110) top is $10\sqrt{2}a_0 \times 6a_0$, as seen in Fig. 1(a) (here, a_0 is the bulk lattice constant). In studying adatom diffusion on the (100) facet, the area of the substrate, the (100)-sloped facet, and the (110) top surface are taken to be $17.5\sqrt{2}a_0 \times 12a_0$, $12a_0 \times 3\sqrt{2}a_0$, and $17.5\sqrt{2}a_0 \times 3.5a_0$, respectively, [see Fig. 1(b)]. The corresponding two model systems contain 6985 and 9721 atoms, respectively. In the studies of dimer, trimer, and tetramer upward diffusion, we enlarge the sizes of the model systems in both the x and y directions accordingly.

To eliminate the possible unphysical effect of using a constant lattice constant in the MD simulations, we first calculate the equilibrium lattice constant at a given temperature using the EAM potentials for both Al and Cu, and then use these temperature-dependent lattice constants in subsequent simulations. Time steps of ~3 and ~3.5 fs for Al and Cu are

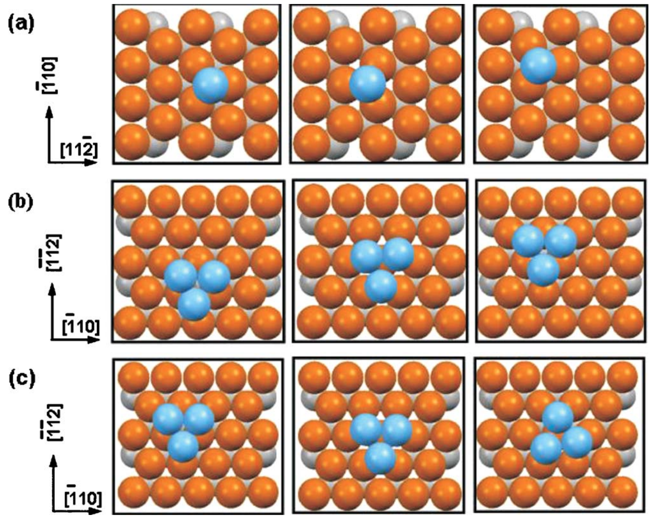

FIG. 2. (Color online) Schematic illustration of the different diffusion mechanisms of an Al adatom and a trimer on Al(111): (a) site-to-site hopping of a single adatom along the (112) direction at 150 K and [(b) and (c)] hopping without rotation and hopping with rotation of a trimer at 350 K.

adopted, and these time steps are fine enough to simulate the dynamic behavior of adatom or cluster diffusion on the facets at the given temperatures. In adopting these time steps, the drifts in the total energy of the systems are less than $10^{-4}\%$. The time duration of the MD simulations ranges from 0.3 to 2 ns, depending on the diffusion rate at given temperatures; such durations are long enough to reveal the atomistic mechanisms of the ascending processes.

III. UPWARD DIFFUSION MECHANISMS OF Al ADATOM ON FACETS OF Al(110)

Before we investigate the upward diffusion behaviors of an adatom and small clusters on the sloped facets of the huts, we first study adatom and small cluster diffusion on flat Al(001), Al(110), and Al(111) in order to elucidate the validity of the EAM potential adopted in our calculations. We use a $5\sqrt{6}a_0 \times 6\sqrt{2}a_0$ cell with a thickness of ten Al layers to study the adatom and cluster self-diffusion. Here, we only present the results of an adatom and a trimer diffusing on a flat Al(111) surface. Figure 2(a) shows the simulation results of the single Al adatom case. For a single adatom, diffusion proceeds via an adatom hopping between two FCC sites through a neighboring HCP site at the temperature of 100 K. Figures 2(b) and 2(c) show different diffusion mechanisms obtained from the MD simulations for a trimer diffusing on Al(111) at 350 K. One is the hopping mechanism from one FCC-H site to another FCC-H site via an HCP-T site; another is the hopping-rotation mechanism, in which the trimer atoms first hop from a FCC-H site to a neighbor HCP-T site, then rotate to a FCC-T site. [In our notation, the trimer with three atoms at fcc sites (FCC) or hcp sites (HCP) and with the mass center at the hollow site (H) or on the top site (T) is labeled as FCC(HCP)-H or FCC(HCP)-T.] Generally, the results are in agreement with previous DFT calculations and MD simulations employing semiempirical potentials.[5,12,36]

To further test the validity of the EAM potential, we also calculate the diffusion coefficient, $D_t = \lambda \Gamma d^2 / 2D$, for Al adatom diffusion on an Al(111) surface. Here, λ is the number of possible hopping directions (three in our case) and Γ is the hopping frequency which is obtained by the hopping number n divided by the total time t. d stands for the jump distance and D for the dimensionality of the diffusion space (two for surface diffusion). The calculated D_t at 150 K is $\sim 4.6 \times 10^{-4}$ cm^2/s, which is also in close agreement with previous study.[5]

Next, we study the diffusion of an Al adatom on the (111)-sloped and (100)-sloped facets of the huts grown on Al(110). We focus our attention on the upward diffusion and convex-edge processes to see if efficient upward diffusion processes can indeed occur. For the (111)-sloped facet, we study the diffusion behaviors of an adatom with a given initial position on the (111)-sloped facet at temperatures ranging from 150 to 750 K with the temperature step of 50 K. Thermal equilibrium can be reached after about 5000 simulation steps (~15 ps) for each simulation, and the independent MD simulations are carried out for several times for a given temperature. At the temperature of 150 K, a single adatom begins to diffuse upward or downward randomly on the (111)-sloped facet. Once the adatom diffuses downward and reaches the concave corner of the facet, it will be trapped and cannot escape from the trap site until the temperature is elevated to above 500 K. However, as the adatom diffuses upward, it can easily cross the convex edge to the top of the hut when the temperature is higher than 150 K. Once on top, the adatom is unable to return downward to the (111)-sloped facet even at the high simulation temperature of 750 K.

Figure 3 (upper panel) shows the concerted exchange mechanism of an adatom diffusing upward from the (111)-sloped facet to the top (110) surface. Figure 3(a-i) gives the initial position of the adatom on the facet, Figs. 3(a-ii)–3(a-iv) exhibit the atomistic diffusion process taking place at the edge of the facet, and Fig. 3(a-v) shows one configuration for a kicked-out edge atom diffusion on the top (110) surface. From the structures obtained in the trajectory of the MD simulations, we found that when the adatom diffuses upward to the convex edge of the facet, it kicks out an edge atom and replaces its position in the edge, while the kicked-out atom becomes an adatom on the top (110) surface. Once the adatom climbs up the huts, it begins to diffuse on the top (110) surface and cannot diffuse downward to the (111) slope facet during all the MD simulations.

Why does the upward and crossing convex-edge diffusion process take place easily? What is so special about (110) surface that produces flattop huts? The special aspect of the fcc(110) surface, in contrast to the (111) and (100) surfaces, is highlighted in Refs. 25 and 26 and also by Fichthorn and Scheffler (Ref. 27): The atomic arrangements at the edges of monatomic steps on fcc(110) are rather loose, making upward diffusion of an adatom via the place exchange mechanism easily accessible. This explanation may also be applied in the present case.

Now, we study Al adatom diffusion on the (100)-sloped facet. We simulate the diffusion process of the adatom with the initial position near the convex edge of the facet at the

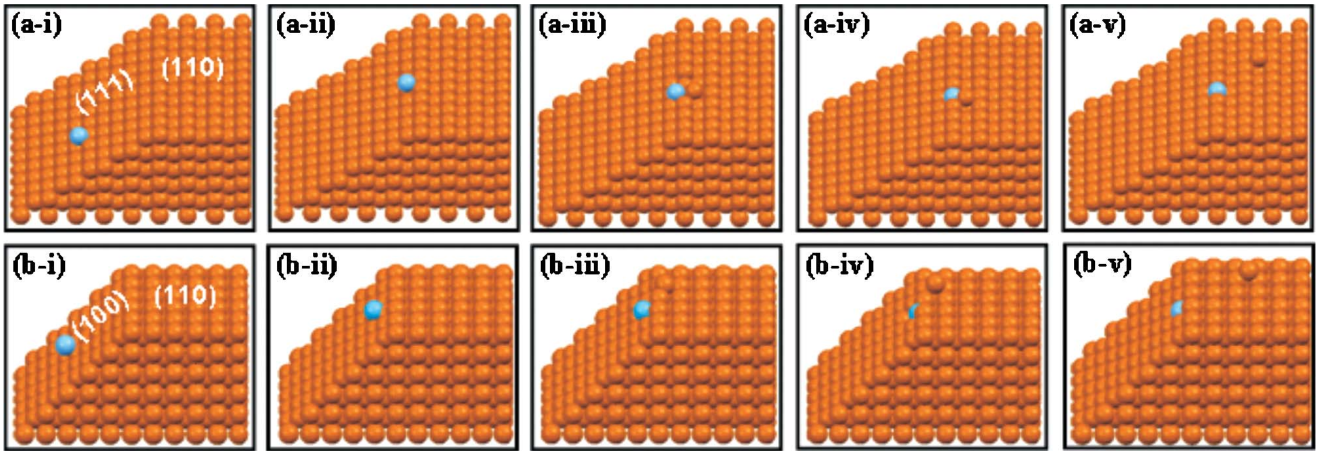

FIG. 3. (Color online) Upper panel: (a-i) initial configuration, (a-ii) and (a-iii) intermediate steps, and (a-iv) final configuration of the concerted exchange mechanism for an Al adatom diffusing upward and crossing the convex edge of the (111)-sloped facet to the top (110) surface at 150 K. Lower panel: (b-i) initial configuration, (b-ii) and (b-iii) intermediate steps, and (b-iv) final configuration of the indirect place exchange mechanism for an Al adatom diffusing upward and crossing the convex edge of the (100)-sloped facet to the top Al (110) surface at 600 K. (a-v) and (b-v) show the configurations after a kicked-out edge atom has diffused to the top (110) surface for the two cases.

temperatures ranging from 500 to 800 K with a temperature step of 50 K, focusing on the upward diffusion and the convex-edge crossing processes. We observe that through a concerted exchange or indirect place exchange mechanism, the adatom can diffuse and cross the convex edge to the top (110) surface. At low temperatures of 500–600 K, the adatom diffuses upward through the concerted exchange mechanism as we discussed above. However, at high temperatures of ~600 K, the adatom can diffuse upward through an indirect place exchange mechanism. Figure 3 (lower panel) shows the process of an indirect place exchange mechanism taking place at the temperature of 600 K. In the indirect place exchange process, the adatom near the convex edge [shown in Fig. 3(b-ii)] first squeezes itself into the surface and pushes its neighboring atom in the second layer of the hut upward to the edge [see Figs. 3(b-iii) and 3(b-iv)], with one edge atom being kicked out. The kicked-out atom moves upward to the top (110) surface and stays on the top surface as an adatom [Fig. 3(b-v)]. Similar to the case of adatom diffusing on the (111)-sloped facet, it is very difficult for the atop adatom to diffuse back to the (100)-sloped facet even at the high simulation temperatures.

Earlier DFT calculations[25,26] of activation energies of an adatom diffusion on the step edge have shown that it is energetically favorable for an adatom to climb up onto the top (110) surface from either the (111)-sloped or (100)-sloped facet, while the energy barrier for an atop adatom to diffuse from the top surface to the sloped facets is large. Our MD simulation results are in agreement with the DFT results; furthermore, these simulations directly elucidated the detailed atomistic mechanisms, including the indirect exchange mechanism not identified in the previous DFT calculations with much smaller supercell sizes.

IV. UPWARD DIFFUSION MECHANISMS OF Al CLUSTERS ON (111) FACET OF Al(110)

To gain a more complete understanding of diffusion processes and growth morphology, it is also desirable to know the diffusion behavior of small clusters of atoms such as dimers, trimers, etc. To this end, we further investigate small cluster diffusion on the (111)-sloped facet of Al(110), focusing on cluster upward diffusion at the step edge of the facets. To simulate the cluster diffusion processes on the facet, here we enlarge the size of the models so that the systems contain more than 20 000 atoms. Our MD simulations begin at the temperature of 300 K, increasing by steps of 50 K in subsequent simulations.

First, we study the case of a dimer diffusing on the (111)-sloped facet. The dimer is put at the center of the facet initially. When thermal equilibrium of the system is achieved after 5000 simulation steps, we find that the dimer can diffuse upward or downward. Once the dimer diffuses downward, it may reach and be trapped at the concave corner of the facet and could not escape from the concave corner even at a high temperature (550 K). Figure 4 shows the snapshots of the simulation results for the dimer upward diffusion process on the (111)-sloped facet at the temperatures of 350 and 450 K, respectively. Figure 4(a-iv) shows the simulation results at the lower temperatures of 300–350 K. Here, we find that the dimer can diffuse upward to a site near the upper edge of the facet, then through a concerted exchange mechanism between one dimer atom and one edge atom, the atom at the edge jumps from the (111)-sloped facet to the top surface. During the process, the dimer is dissociated into two adatoms and one of them replaces the edge atom being kicked out and placed on top. The other atom of dimer then may experience the same diffusion processes of an adatom as studied in the previous section. Finally, the two atop adatoms associate and form a new dimer on the top (110) surface [Fig. 4(a-v)]. The new dimer can easily diffuse on the top (110) surface at the simulation temperature, but the descending diffusion process of the dimer from the top (110) surface to the (111)-sloped facet is not found during simulations.

At high temperatures of 400~550 K, our MD simulations show that a dimer diffuses upward and then directly place exchanges two neighboring edge atoms as a whole

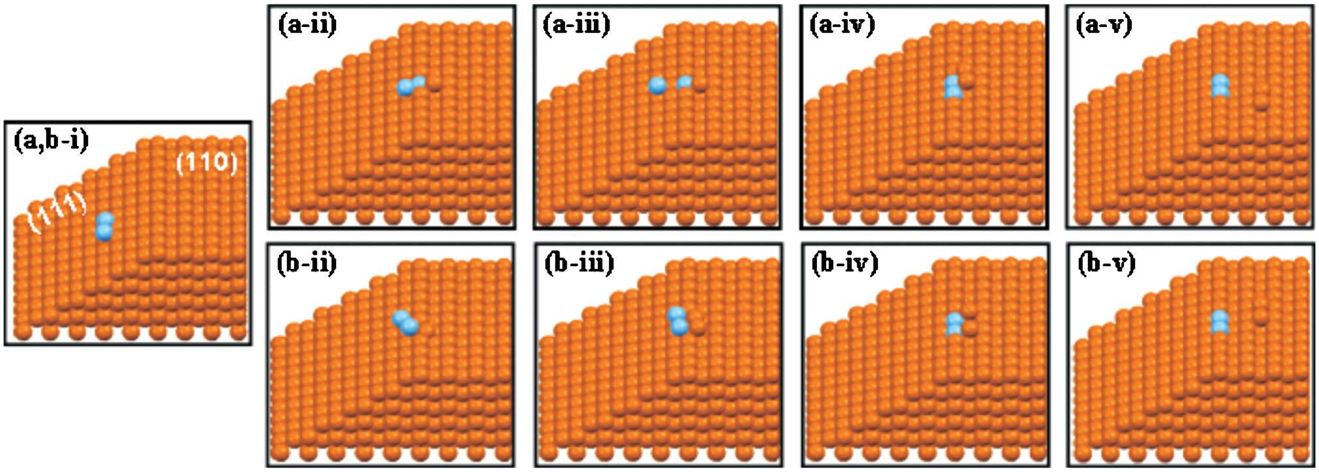

FIG. 4. (Color online) (a-i) and (b-i) common initial configuration of an Al dimer diffusing upward and crossing the convex edge of the (111)-sloped facet to the top (110) surface at 350 K. Upper panel: (a-ii) and (a-iii) intermediate steps and (a-iv) final configuration of the sequential concerted exchange mechanism at 350 K. Lower panel: (b-ii) and (b-iii) intermediate steps and (b-iv) final configuration of the exchange mechanism of the dimer as a unit at 400 K. (a-v) and (b-v) show the configurations after a dimer formed by two kicked-out edge atoms has diffused to the top (110) surface for the two cases.

unit. The two kicked-out edge atoms move to the top (110) surface and form a new dimer [Figs. 4(b-ii)–4(b-v)].

Next, we study trimer upward diffusion toward the top (110) surface. We find that a trimer can also diffuse upward from the (111)-sloped facet to the top (110) as the temperature increases to 500 K. However, in the temperature range of our simulations, the trimer always dissociates at the edge through the concerted exchange mechanism shown in Fig. 5. Thus, for a trimer, massive atom transportation to the top (110) surface can be realized via the concerted exchange mechanism in which the trimer dissociates into one atom and one dimer.

For tetramer diffusion on the (111)-sloped facet, our simulations show that it can also diffuse upward at the temperature of about 500 K, and at the convex edge of the (111)-sloped facet, the tetramer may dissociate into two dimers (Fig. 6, upper panel) or one atom and one trimer (Fig. 6, lower panel). In the former case, one dimer from the dissociated tetramer may exchange directly with the two edge atoms, and the kicked-out edge atoms move to the top surface of the hut and stay there as an ad-dimer, while the other dimer is left on the facet near the edge, experiencing a similar process for dimer diffusion. In the latter case (Fig. 6, lower panel), one atom from the dissociated tetramer replaces one convex-edge atom. The remaining trimer on the (111)-sloped facet may then undergo the same diffusion processes of a trimer discussed earlier.

Briefly, we summarize the diffusion behaviors of clusters on the (111)-sloped facet observed in our MD simulations at the temperatures ranging from 350 to 500 K. We found that a dimer, trimer, or tetramer can all diffuse upward on the (111)-sloped facet, and then through a combined process of cluster dissociation and place exchange between the cluster and hut edge, atoms are transported to the top surface of the hut, leading to hut growth. Cluster dissociation at the step edge has been observed in previous MD study of cluster downward diffusion,[20] and the dissociation of a dimer at the step edge could be attributed to shear motion[39] as well as a short-range attraction effect.[40] The different temperature dependences we observed in the upward diffusion of small clusters with different sizes can be understood from the calculated dependence of the diffusion on the cluster size.[10]

V. UPWARD DIFFUSION MECHANISMS OF Cu ADATOM AND CLUSTERS ON FACETS OF Cu(110)

In order to explore the potentially generic nature of the kinetic processes discussed above, we have further per-

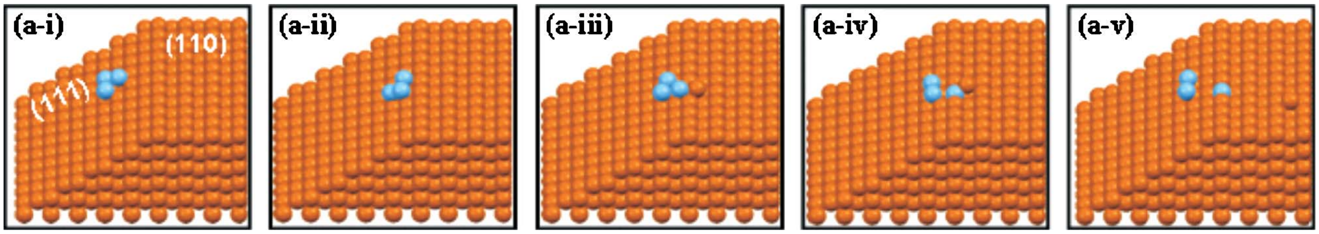

FIG. 5. (Color online) Different kinetic steps of the dissociation and concerted atom exchange mechanism of an Al trimer crossing the convex edge of a (111)-sloped facet at 500 K.

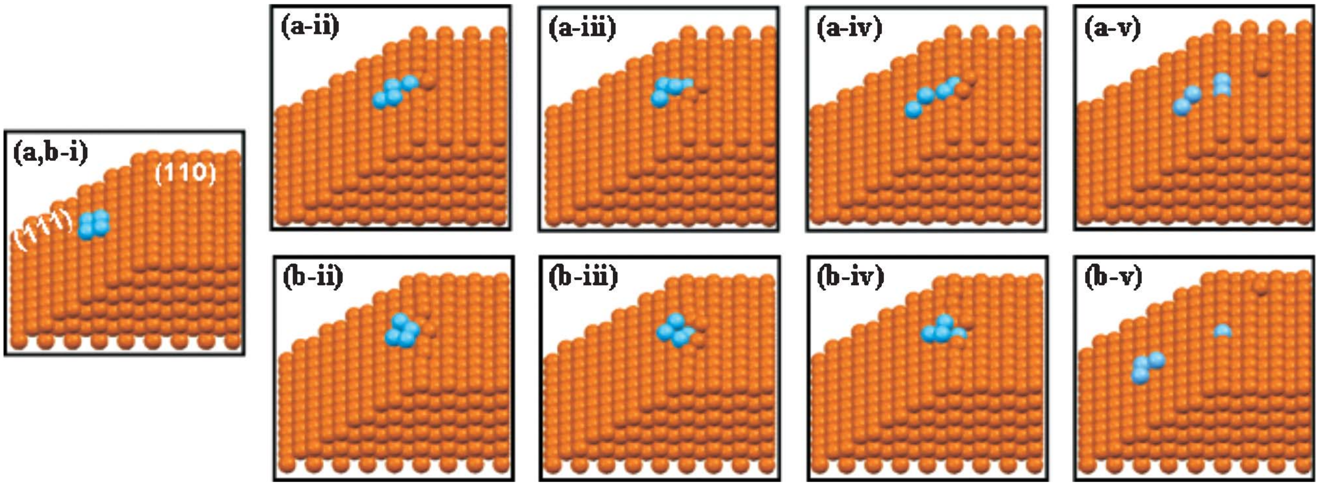

FIG. 6. (Color online) Kinetic steps of an Al tetramer diffusing upward and crossing the convex edge of the (111)-sloped facet to the top (110) surface by a combination of different dissociation and concerted exchange mechanisms. At 500 K (upper panel), the tetramer dissociates into two dimers at the edge, while at 600 K (lower panel), it dissociates into one atom and one trimer.

formed MD simulations of Cu adatom and cluster upward diffusion on sloped facets of Cu(110). Similar to the cases of Al, all the kinetic processes identified above have been observed for Cu, but for each case a relatively higher temperature is needed. For example, for a single Cu adatom or a Cu-Cu dimer diffusing up to the top Cu(110) surface from a sloped Cu(111) facet, the minimum simulation temperature had to be 400 and 500 K, respectively. These observations are consistent with the fact that on a Cu surface, the corresponding kinetic processes have higher activation barriers than that on Al.[5] Overall, the MD simulation results for both Al and Cu suggest that the formation of hut islands observed in Al(110) homoepitaxy[26] should also be expected to occur in homoepitaxial growth of Cu(110) and other fcc metal (110) surfaces under proper growth conditions.

VI. SUMMARY

In summary, we have studied upward self-diffusion of adatoms and small clusters on faceted huts formed in fcc metal (110) homoepitaxy using molecular dynamics simulations with interatomic potentials described by the embedded-atom method (EAM). Our results showed that both individual adatoms and small clusters on the (111) and (100) faces of the huts on Al and Cu(110) can readily diffuse upward and cross the convex edges of the huts, but with different atomistic mechanisms. An adatom can cross the convex edges via a simple concerted exchange or indirect place exchange mechanism. In contrast, the upward diffusion and convex-edge crossing of small clusters can be realized by their dissociation at or near the edges of the hut after one or two atoms belonging to the cluster are incorporated into the edges. These results are in agreement with the previous first-principles calculations and experimental observations and also lead to the identification of new kinetic processes of long-range nature. Overall, the present simulation studies revealed that there truly exists efficient upward mass transport on faceted islands in fcc metal (110) homoepitaxy, and such upward diffusion processes are expected to play a key role in defining the kinetic faceting instability in these growth systems.

ACKNOWLEDGMENTS

We are grateful to Biao Wu, Wenguang Zhu, Songyou Wang, and Shunfang Li for helpful discussions. We also thank Hua Chen for a critical reading of the paper. This work has been supported by the National Science Foundation of China under Grant No. 10574113 (Y.J.), by the U.S. National Science Foundation under Contract No. DMR-0606485 (Z.Z.), and in part by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under Contract No. DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC.

---

[1] Z. Y. Zhang and M. G. Lagally, Science **276**, 377 (1997).
[2] J. E. Black and Z. J. Tian, Phys. Rev. Lett. **71**, 2445 (1993).
[3] M. Karimi, T. Tomkowski, G. Vidali, and O. Biham, Phys. Rev. B **52**, 5364 (1995).
[4] R. Stumpf and M. Scheffler, Phys. Rev. B **53**, 4958 (1996).
[5] N. I. Papanicolaou, V. C. Papathanakos, and D. G. Papageorgiou, Physica B **296**, 259 (2001).
[6] Oleg Trushin, Altaf Karim, Abdelkader Kara, and Talat S. Rahman, Phys. Rev. B **72**, 115401 (2005).
[7] Altaf Karim, Ahlam N. Al-Rawi, Abdelkader Kara, Talat S. Rah-

man, Oleg Trushin, and Tapio Ala-Nissila, Phys. Rev. B **73**, 165411 (2006).

[8] P. J. Feibelman, Phys. Rev. Lett. **65**, 729 (1990).

[9] H. J. Ernst, F. Fabre, R. Folkerts, and J. Lapujoulade, Phys. Rev. Lett. **72**, 112 (1994).

[10] S. Ovesson, A. Bogicevic, and B. I. Lundqvist, Phys. Rev. Lett. **83**, 2608 (1999).

[11] R. Stumpf and M. Scheffler, Phys. Rev. Lett. **72**, 254 (1994).

[12] C. M. Chang, C. M. Wei, and S. P. Chen, Phys. Rev. Lett. **85**, 1044 (2000).

[13] G. L. Kellogg and A. F. Voter, Phys. Rev. Lett. **67**, 622 (1991).

[14] X. Wei, P. A. Greaney, and D. C. Chrzan, Phys. Rev. B **70**, 033402 (2004).

[15] J. Jacobsen, K. W. Jacobsen, P. Stoltze, and J. K. Nørskov, Phys. Rev. Lett. **74**, 2295 (1995).

[16] G. L. Kellogg and P. J. Feibelman, Phys. Rev. Lett. **64**, 3143 (1990).

[17] Z. J. Tian and T. S. Rahman, Phys. Rev. B **47**, 9751 (1993).

[18] B. D. Yu and M. Scheffler, Phys. Rev. Lett. **77**, 1095 (1996).

[19] Y. G. Li, T. J. Raeker, and A. E. DePristo, Phys. Rev. B **50**, 14742 (1994).

[20] G. Ehrlich and F. G. Hudda, J. Chem. Phys. **44**, 1039 (1966).

[21] R. L. Schwoebel and E. J. Shipsey, J. Appl. Phys. **37**, 3682 (1966).

[22] J. Villain, J. Phys. I **1**, 19 (1991).

[23] H. C. Huang and J. Wang, Appl. Phys. Lett. **83**, 4752 (2003).

[24] S. J. Liu, E. G. Wang, C. H. Woo, and H. C. Huang, J. Comput.-Aided Mater. Des. **7**, 195 (2001).

[25] F. Buatier de Mongeot, W. Zhu, A. Molle, R. Buzio, C. Boragno, U. Valbusa, E. G. Wang, and Z. Y. Zhang, Phys. Rev. Lett. **91**, 016102 (2003).

[26] W. Zhu, Francesco Buatier de Mongeot, U. Valbusa, E. G. Wang, and Z. Y. Zhang, Phys. Rev. Lett. **92**, 106102 (2004).

[27] K. Fichthorn and M. Scheffler, Nature (London) **429**, 617 (2004).

[28] M. S. Daw and M. I. Baskes, Phys. Rev. Lett. **50**, 1285 (1983).

[29] A. F. Voter and S. P. Chen, Symposia Proceedings No. 82 (Materials Research Society, Pittsburgh, 1987), p. 175.

[30] A. F. Voter, in *Intermetallic Compounds: Principles and Practice*, edited by J. H. Westbrook and R. L. Fleischer (Wiley, New York, 1995), Vol. 1, p. 77.

[31] R. A. Johnson, Phys. Rev. B **37**, 3924 (1988).

[32] R. A. Johnson, Phys. Rev. B **39**, 12554 (1989).

[33] B.-J. Lee, J.-H. Shim, and M. I. Baskes, Phys. Rev. B **68**, 144112 (2003).

[34] S. D. Borisova, G. G. Rusina, S. V. Eremeev, G. Benedek, P. M. Echenique, I. Yu, Sklyadneva, and E. V. Chulkov, Phys. Rev. B **74**, 165412 (2006).

[35] V. B. Shenoy, Phys. Rev. B **71**, 094104 (2005).

[36] Z. G. Xia, D. Y. Sun, M. Asta, and J. J. Hoyt, Phys. Rev. B **75**, 012103 (2007).

[37] Y. L. Bouar and F. Soisson, Phys. Rev. B **65**, 094103 (2002).

[38] A. Bogicevic, S. Ovesson, B. I. Lundqvist, and D. R. Jennison, Phys. Rev. B **61**, R2456 (2000).

[39] Z. P. Shi, Z. Y. Zhang, A. K. Swan, and J. F. Wendelken, Phys. Rev. Lett. **76**, 4927 (1996).

[40] J. G. Yu and J. G. Amar, Phys. Rev. Lett. **89**, 286103 (2002).