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Rapid decay of vacancy islands at step edges on Ag(111): step orientation dependence

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Abstract

Previous work has established that vacancy islands or pits fill much more quickly when they are in contact with a step edge, such that the common boundary is a double step. The present work focuses on the effect of the orientation of that step, with two possibilities existing for a face centered cubic (111) surface: A- and B-type steps. We find that the following features can depend on the orientation: (1) the shapes of islands while they shrink; (2) whether the island remains attached to the step edge; and (3) the rate of filling. The first two effects can be explained by the different rates of adatom diffusion along the A- and B-steps that define the pit, enhanced by the different filling rates. The third observation—the difference in the filling rate itself—is explained within the context of the concerted exchange mechanism at the double step. This process is facile at all regular sites along B-steps, but only at kink sites along A-steps, which explains the different rates. We also observe that oxygen can greatly accelerate the decay process, although it has no apparent effect on an isolated vacancy island (i.e. an island that is not in contact with a step).

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Nanoscale islands of adatoms or vacancies on metal surfaces are intrinsically metastable, and often decay on timescales of a few minutes to a few hours at typical experimental temperatures. Studies of their collective and individual evolution have provided rich insights into the mechanisms and energetics of processes at metal surfaces [1, 2]. For instance, it was discovered that rather large islands can, under certain circumstances, move substantial distances via a mechanism now known as periphery diffusion [3–5]. In 1998, a surprising effect was reported [6], in which an island shrinks and disappears much more quickly after it moves into ‘contact’ [6–10] with another step edge, in such a way that the contact border is twice as high as the border of the original island itself. (This geometry is illustrated in figure 1(A).) Several possible reasons have been suggested for this acceleration [7–13]. The acceleration has been observed

both for adatom islands in contact with a descending step {on Cu(111) and Ag(111)}, and for vacancy islands (also called pits) in contact with an ascending step {on Ag(111)}. The latter geometry is illustrated in figure 1(B).

In this paper, we report some new observations regarding the evolution of pits after they move into contact with an ascending step edge on Ag(111). We find that pits decay at different rates, and adopt different shapes and positions during decay depending on step orientation. We will explain these features in terms of atomic arrangements at the step edges.

Thus, it is important to note that there are two types of close-packed step edges on Ag(111). These are known as A-type and B-type steps, and they lie along close-packed directions. They are illustrated in figure 8 of [13], in figure 5 of [14], or in figures 6 and 7 presented later in this paper. On the (111) surface of an fcc system such as Ag, all parallel close-packed steps that change the elevation of terraces in the same way (i.e. up-going or down-going) are of the same

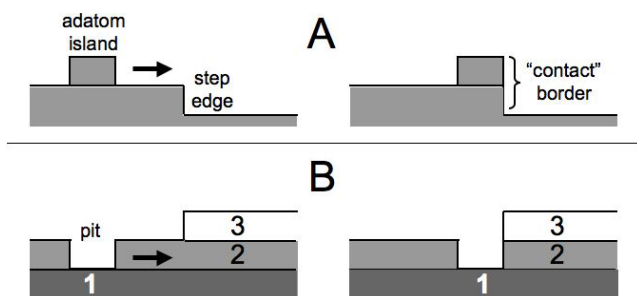


Figure 1. Schematic cross-sections: (A) adatom island approaching step edge; and (B) vacancy island approaching step edge. Numbers in (B) define levels that are referenced throughout the paper, always starting with one as the floor of the pit. Note that previous work has shown that step edges need not align perfectly (as shown for simplicity in figure 1) in order for accelerated coarsening to occur, but rather can be separated by several lattice constants [7].

type. The A-type steps can be thought of as (100) microfacets, exhibiting quasi-fourfold hollow sites, and the B-type steps as (111) microfacets, exhibiting quasi-threefold hollow sites. The A- and B-type step energies are nearly equal on Ag(111) [13]. Nonetheless, there can be observable distinctions between the two types of steps. Of particular relevance to this paper is the fact that adatoms diffuse faster along A-steps than along B-steps on Ag(111) [11, 13, 15, 16]. This is supported by effective medium theory (EMT) calculations, which predict diffusion barriers of 0.222 eV and 0.300 eV along A- and B-steps, respectively [16], which corresponds to $20\times$ faster diffusion along A-steps at 300 K. The same trend is predicted by the embedded atom method (EAM), which yields estimates of 0.294 eV and 0.338 eV, respectively [13], corresponding to $5.5\times$ faster diffusion along A-steps.

2. Experimental details

The Ag(111) single crystal sample was cleaned by repeated cycles of Ar^+ sputtering (15–30 min, 20 mA, 1.0–1.5 kV, $T = 300$ K) followed by annealing at ~ 525 K until no impurities could be detected by Auger electron spectroscopy (AES). The STM morphology was monitored after the sample had cooled to room temperature. With this preparation regimen, vacancy islands introduced by sputtering could still be observed occasionally on the surface immediately after annealing. Typical tunneling conditions were +1.5 V and 1.0 nA.

The orientation of this sample was the same as in our previous studies of Ag(111) [14, 17]. Hence, results from the previous studies allowed us to identify A- and B-step orientations in the present work. Specifically, it is well-established that the dendritic islands formed by Ag deposition at 120–135 K display prominent triangular envelopes, in which the edges of the triangles are B-steps. Thus, we could establish step orientations from our previous experimental observations [14] of dendritic Ag island formation on this substrate. This assignment was reinforced by our previous study of sulfur on Ag(111) [18], wherein we observed that terrace steps facet selectively at low coverages of sulfur. We

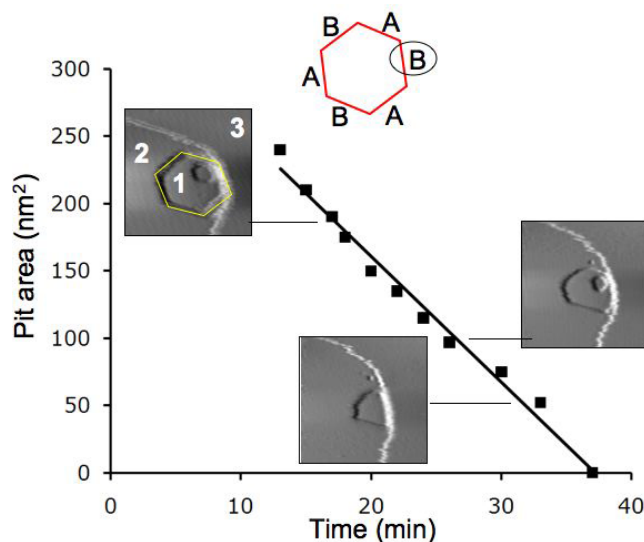


Figure 2. Room temperature pit decay with ascending B-step. All STM images are $30\text{ nm} \times 30\text{ nm}$. Terraces are labeled by level number, after figure 1(B).

assigned the preferred orientation as the A-step, since adsorbed sulfur binds most strongly at fourfold hollow sites.

In previous work, it has been determined that the acceleration of decay of adatom islands can already occur when the typical or mean local separation of an island from the adjacent step edge is reduced to a few lattice constants [7]. In our experiments, the STM resolution was not sufficient to determine the minimum distance for effective contact.

3. Results

Figure 2 shows the decay (i.e. filling) of a vacancy island, containing about 3650 vacancy sites, in contact with a B-step. It encloses a much smaller vacancy island, but this does not affect decay of the larger vacancy island. Based on the linear least-squares fit shown by the solid line, the initial decay rate, R , is $\sim 9.3\text{ nm}^2\text{ min}^{-1}$. Measurements of several pits, with initial sizes ranging from 2628 to 3735 vacancy sites, in contact with B-steps show that the initial rate consistently is in the range $9.3\text{--}9.6\text{ nm}^2\text{ min}^{-1}$. For comparison, the decay rate of this vacancy island (and others observed in this study) when not in contact with a step edge is $R \leq 0.15\text{ nm}^2\text{ min}^{-1}$.

In figure 2, note that the vacancy island in contact with a B-step retains a rather round shape as it shrinks, and that the border between the pit and the ascending step remains quite long, compared with the approximate diameter of the island. Further, the vacancy island does not move away from the step edge.

Figure 3 shows the decay of a vacancy island, containing about 3180 vacancy sites, when it approaches a pair of adjacent, ascending A-step edges on the clean Ag(111) surface. There are two stages in the filling of the pit. Between 0 and 25 min, the pit shrinks at a rate of $\sim 4.1\text{ nm}^2\text{ min}^{-1}$, based on the linear least-squares fit to the data shown by the

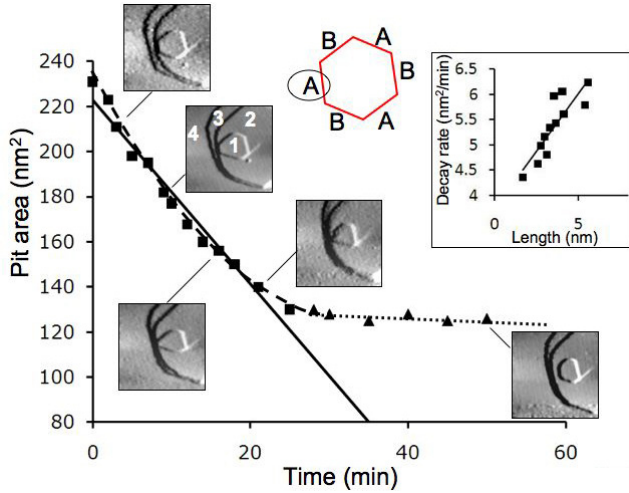


Figure 3. Room temperature pit decay with ascending A-step. All STM images are $50 \text{ nm} \times 50 \text{ nm}$. Terraces are labeled by level number, after figure 1(B).

solid line. This is slightly less than half the rate near a B-step (cf figure 2). In this period, the two ascending steps approach and merge. Simultaneously, the bottom pit becomes increasingly triangular, as its A-steps shorten relative to its B-steps. The second stage begins after about 25 min, when the pit shrinks at a much slower rate of $0.15 \text{ nm}^2 \text{ min}^{-1}$ —lower by a factor of ~ 27 than the initial rate. In this second stage, the pit moves away from the ascending step and evolves back toward a hexagonal shape.

Measurements of islands with initial sizes ranging from 490 to 3180 vacancies consistently show that they fill at a rate of $4.0\text{--}4.1 \text{ nm}^2 \text{ min}^{-1}$ when they touch A-steps.

Figure 4 shows a situation where a pit first comes close to an A-step. Shortly thereafter, it also comes close to a B-step (at the upper left of the pit), either due to cluster migration or step edge motion, or both. The decay rate is initially $4.1 \text{ nm}^2 \text{ min}^{-1}$ along the A-step (solid line, and data points from 0 to 8 min), but it changes to $9\text{--}11 \text{ nm}^2 \text{ min}^{-1}$ along the B-step (dashed line, and data points from 22 to 33 min), which again shows the difference in kinetics for the two step orientations.

Thus far, decay rates have been based on linear least-squares fits to the decrease of pit area with time. However, one might argue that the decay rate, R , should not be strictly constant, but rather should depend on the length, L , of the interface in common with the pit and the extended step. In the simplest picture of static straight steps in perfect contact, one might expect that the decay rate is proportional to this length, i.e., $R = cL$. In other words, $R(L)$ should be a straight line passing through the origin. The inset to figure 3 indicates that $R(L)$ is indeed close to linear, but $R(L)$ is best fit by a line that does not intercept the origin, i.e. $R = 0.42L + 3.75$ (with R in $\text{nm}^2 \text{ min}^{-1}$ and L in nm). Furthermore, we find that L decreases linearly with time—if one neglects step edge fluctuations—according to $L = 5.6 - 0.19t$ (L in nm, t in min). This, together with the observed form of $R(L)$, is used to construct the quadratic fit to pit area versus time shown in figure 3 for the regime $t < 27 \text{ min}$ where $L > 0$. We set R

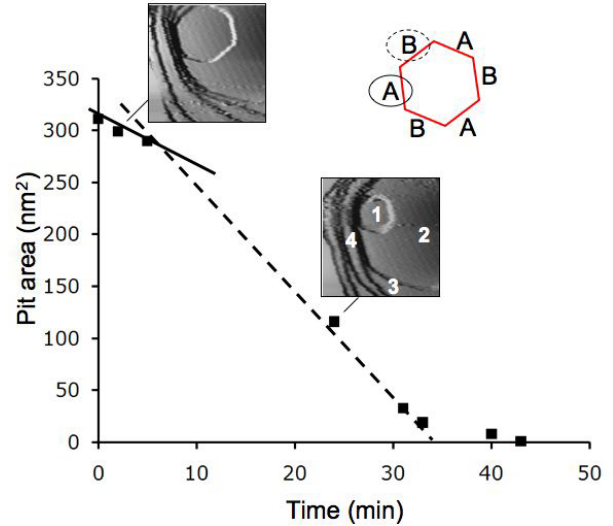


Figure 4. Room temperature pit decay, in which a vacancy island first comes into contact with an A-step, then comes close to a B-step, during decay. All STM images are $40 \text{ nm} \times 40 \text{ nm}$. Terraces are labeled by level number, after figure 1(B).

equal to a small constant value once the island has detached, producing the linear fit shown in figure 4 for $t > 27 \text{ min}$.

We do not expect the empirically determined linear fit to $R(L)$, shown in figure 3 inset, to apply for all $L > 0$. The exact $R(L)$ presumably is significantly below the linear best fit through the data for small enough L ; in fact, we know that R should be $\sim 0.15 \text{ nm}^2 \text{ min}^{-1}$ for $L = 0$ (a detached pit). With regard to the deviation from a simple proportionality $R = cL$, one possible contribution is the fact that atoms filling the pit can come from sites on the upper step edge which are not within the contact border. See the following discussion. Another possible contribution arises from the fact that the steps are dynamic rather than static, with communication between nearby separated step edges facilitated by fluctuations [19]. A complete understanding of $R(L)$ would be a suitable subject for future investigations.

Finally, figure 5 shows the decay of a vacancy island while the chamber is backfilled with oxygen to a pressure of $8 \times 10^{-10} \text{ Torr}$. At first, the pit is not close enough to the ascending step edge, and suffers almost no change in its area. When the pit touches the ascending A-step, it suddenly begins to shrink at a rate of $63 \text{ nm}^2 \text{ min}^{-1}$, and continues until it disappears. This rate is higher than without oxygen, by a factor of ~ 16 .

4. Discussion

Our goal is to develop a qualitative model that explains three experimental observations for the clean surface: (1) pits can assume different shapes as they shrink along ascending step edges—truncated triangles with short borders along A-steps, and rounder shapes with longer borders along B-steps; (2) pits may detach from A-steps, but they remain bound to B-steps; and (3) the rate of filling is faster along B-steps than along A-steps (by about a factor of 2).

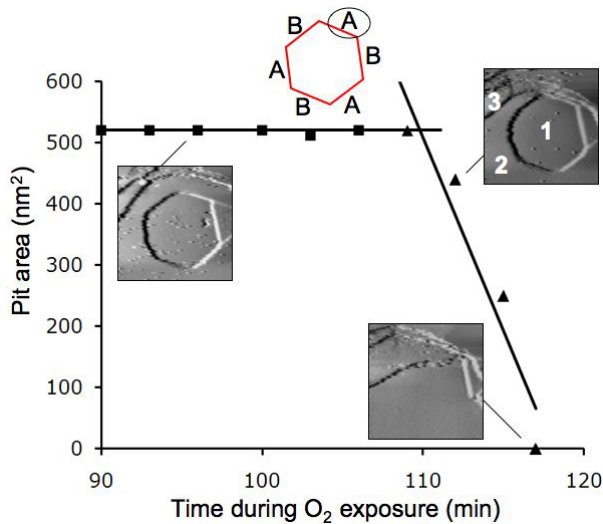


Figure 5. Decay of a pit at room temperature in oxygen gas at 8×10^{-10} Torr. The pit is adjacent to an A-step. All STM images are $40 \text{ nm} \times 40 \text{ nm}$. Terraces are labeled by level number, after figure 1(B).

Figures 6(a)–(c) represent a model that qualitatively explains the first two features. A simple and compelling argument for the observed behavior is that when adatoms enter the pit, their residence time on B-steps is longer than on A-steps, making it more likely that a new row of atoms can nucleate along the B-step edge. This leads to preferential growth—filling—perpendicular to the B-steps of the pit. We note parenthetically that these differences in edge diffusion have also been argued to influence island growth shapes during deposition⁵.

In figure 6(b), the filled gray circles correspond to atoms that have partially filled the pit, after the vacancy island has touched an (imaginary) ascending B-step edge on the right-hand side. Due to the slow migration of atoms along the B-step at the island-step boundary, these atoms nucleate and grow a new line of atoms along the B-step. Consequently, the boundary between the island and the ascending B-step remains quite long, consistent with the experimental data (figure 2).

As shown in figure 6(c), when the vacancy island touches an (imaginary) ascending A-step on its left, the filling atoms tend to find and stick to the two closest B-steps. This leads eventually to a triangular pit shape—although the two corners of the triangle farthest from the ascending step are truncated, exactly as in experiment (figure 3). When the B-steps converge at the border with the ascending step, there is essentially no remaining linear boundary between the pit and the step edge, and the pit may diffuse away from the ascending step edge, as seen in figure 3.

It should be noted that another process must occur, in addition to those described above. That is crossover of step edge atoms, by periphery diffusion, between A- and B-type

⁵ For island growth in fcc(111) homoepitaxy, deposited atoms are fed to all island edges. Slower edge diffusion should lead to an excess edge atom density at B-steps. In the absence of other factors, this would produce a net flux from B to A-steps, and faster growth perpendicular to A-steps. However, the situation in pit filling is very different, with adatoms fed into the pit at just one edge.

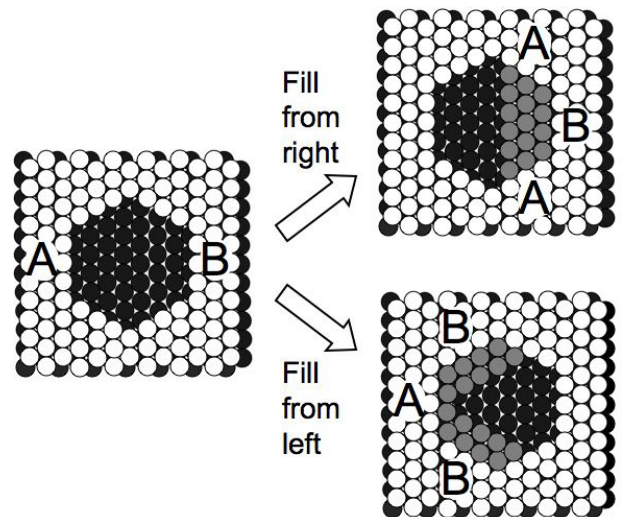


Figure 6. Schematic model for filling of vacancy islands.

(a) Hexagonal pit in a terrace. Darkest circles in the middle hexagon represent atoms at the floor of the pit (level 1 of figure 1(B)), and white circles are atoms in the surrounding terrace (level 2). (b) The result when the pit touches a B-step on its right perpendicular edge. (c) The result when the pit touches an A-step on its left perpendicular edge. In (b) and (c), intermediate gray circles are atoms in level 2 that fill the pit. The step that the pit touches is not shown. Levels are defined in figure 1(B).

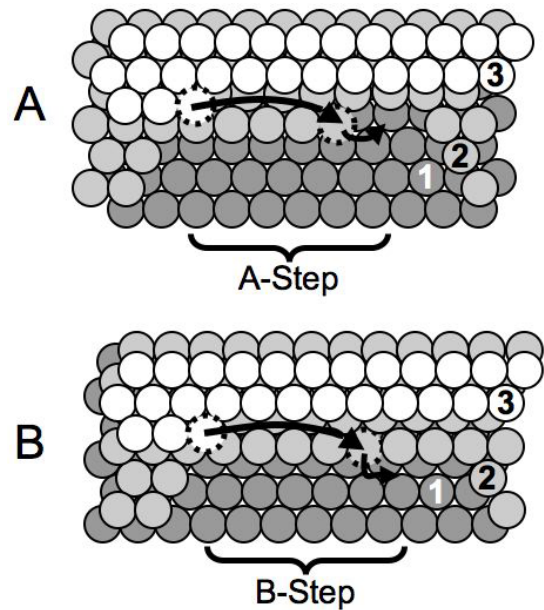


Figure 7. Schematic model for the concerted exchange mechanism at (A) a kink site on an A-step, and (B) a regular site on a B-step. In both cases, an atom detaches from a kink site along a step in level 3 (dashed white circle), diffuses along the step edge, and eventually pushes out an atom along a step edge in level 2 (dashed, light gray circle). Levels are defined in figure 1(B).

step edges. (Another possible process—detachment from the pit edge, followed by diffusion of atoms across the ‘terrace’ at the bottom of the pit, and reattachment at a step edge—is likely to be negligible [20].) Indeed, facile diffusion along and crossover between adjacent A- and B-steps is well supported

by a number of aspects of the experimental data. Perhaps most striking is the ability of the pits to reshape, e.g. from a truncated triangle toward a hexagon in figure 3. It is also supported by the well-known ability of vacancy islands to diffuse via perimeter diffusion in this system [3–5]. However, it appears that the exchange between B and A-steps is not so fast that it erases the differences in the characteristics of the pits as they fill, which are observed in the experiments and highlighted in figure 6.

In this context, it is noteworthy that another factor acts in concert with the anisotropy in edge diffusion. Recall that pits at extended B-steps fill twice as fast as those at A-steps. Thus, in the former case, there is less time during filling for adatoms to be transported away from the common B-step around the pit periphery. In contrast, the slower rate of filling for a pit approaching an A-step facilitates transport away from the common A-step to the neighboring B-steps. Thus, the difference in filling rates enhances the effects of slower diffusion along B-steps.

The third experimental observation to be explained is the difference in filling rates itself. The explanation must be formulated in view of the general mechanism underlying rapid decay of pits (or islands) in contact with an extended step edge. As a prelude, we should first describe the more conventional picture of pit filling. With reference to the left side of figure 1(B), it is this: atoms detach from a step edge in the upper layer (level 3), diffuse across the terrace (level 2), and descend the edge of the pit to the lower layer (level 1) after surmounting an Ehrlich–Schwoebel (ES) step edge barrier. With this in mind, several mechanisms have been proposed for accelerated decay at terrace steps [7–13], including reduction of the ES barrier due to quantum confinement of electronic surface states, reduction of the ES barrier due to a concerted exchange pathway, and circumvention of the step detachment barrier, also due to a concerted process. A key component of both the second and third mechanisms is the feature that steps are dynamic, their fluctuations enabling local near-contact of step edges as pointed out originally by Giesen *et al* [6]. This near-contact can enable various concerted processes. We favor the third picture, which was initially proposed by Morgenstern *et al* [8, 11]. Their key idea is that downward mass transport which results in pit filling occurs via a concerted ‘exchange and push-out’ process involving atoms at nearby portions of step edges in adjacent layers (levels 2 and 3 in figure 1(B)). The upper level atom (in level 3) never fully detaches from the upper step edge before starting to pushing out the lower level atom (in level 2) to take its place. Thus, a relatively high degree of coordination (bonding) of the atoms is retained throughout. This is not the case for hopping over the step edge. Thus, concerted atom transfer is like ‘passing the baton’ where contact is maintained between the runners throughout the process.

To understand why the decay rate depends on step orientation for the concerted mechanism, it is instructive to recall results from a previous analysis of the conventional ES barrier for interlayer transport of an isolated adatom [21]. It was found that the *local orientation* of the step determines whether exchange is favored over hopping down. Exchange is favored at straight B-steps or at kinks on A-steps, both

cases corresponding to (111) microfacets. For this geometry, an atom in the lower layer can be easily pushed out through a bridge site between two atoms in the supporting layer. In contrast, for straight A-steps or kinks on B-steps, the atom being extruded must pass over or nearly over an on-top site, and this is associated with a higher barrier. Although the issue in this paper is not the interlayer transport of an isolated adatom, but rather interlayer transport of an atom embedded in a step edge, the same geometric considerations apply. EMT calculations in [11] support this view.

A schematic of the processes in facile downward transport at nearby step pairs is provided in figure 7. Typically, an atom will detach from a kink in the upper layer step edge (level 3), diffuse along the upper step edge, and then undergo facile exchange-mediated downward transport anywhere along a B-step, but preferentially at kinks on A-steps. The more restricted exchange in the latter case presumably produces the slower rate observed for pit filling when contact is made along A-steps. The effective barrier for the process, E_{rapid} , is given by the sum of: (i) the energy cost to form an atom on the straight step by extraction from the kink site; and (ii) the barrier for exchange [11]. Barrier (i) is—to a good approximation—the nearest-neighbor interaction of $\varphi \sim 0.2$ eV, which controls the equilibrium population of isolated edge atoms along a step of either orientation, A or B. Barrier (ii) is the barrier for the concerted exchange process at the step in level 2. Our key argument is that this barrier is lower at an extended, straight B-step than at an extended, straight A-step.

Another general issue that should be considered is the relative motion of the pit and the step edge during filling. As material is removed from the upper extended step (level 3), the step should recede from the pit, at least locally. Likewise, as material is added to the pit, its edge should advance away from the extended step. One might imagine that these effects would immediately inhibit pit filling. However, regarding motion of the extended step, removal of material will certainly create a local indentation and thus local recession. However, periphery diffusion along this extended step will tend to fill this indentation, thus restoring the extended step to its original position. Such response of a step edge to local erosion has been observed in other studies [22, 23]. In addition, elastic effects between nearby step edges have been shown to hold the pit and the step edge together [11].

Our explanations for the differences between pit filling at A-steps and B-steps call for quantitative modeling in future studies. An atomistic approach such as kinetic Monte Carlo (as opposed to a continuum approach) would undoubtedly be most appropriate, since other authors [24, 25] have demonstrated that decay of very small features, like the vacancy islands described in this paper, can only be described correctly using an atomistic approach.

Turning to the acceleration induced by oxygen, it is striking that the pit does not change measurably until it touches a step edge (figure 5), and then the effect of oxygen is to accelerate the filling process by a factor of about 16. It is known that adsorbed oxygen accelerates decay of adatom islands on Ag(100) [26, 27], and of Ag(111)-like mounds in thick films [28]. Clearly, it exerts a similar effect on the decay

of pits at step edges. At this time, we are not able to offer a detailed explanation.

5. Conclusions

Previous work has established that islands of adatoms and vacancies fill much more quickly when they are in contact with a descending or ascending step edge, respectively, than when they are in the middle of a terrace. The present work focuses on the effect of step edge orientation. For vacancy island decay at ascending steps on clean Ag(111), we find that the following features can depend on the orientation of the contact boundary: (1) the shapes of islands while they shrink; (2) whether the island remains attached to the step edge; and (3) the rate of filling, with the rate being twice as fast along a B-step than an A-step. The first two effects can be explained by the different rates of adatom diffusion along A- and B-type steps of the pit, enhanced by the different filling rates. The third observation—the difference in the filling rate itself—is explained within the context of the concerted exchange mechanism at a nearby pair of steps, previously suggested by Morgenstern *et al* [11]. We propose that the transition state for this process is favorable at all regular sites along B-steps, but only at kink sites along A-steps, which explains the different rates. We also observe that oxygen can greatly accelerate the process, although it has no apparent effect on decay of an isolated vacancy island (i.e. a pit that is not in contact with an ascending step).

Acknowledgments

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