Hybrid Monte Carlo–molecular dynamics algorithm for the study of islands and step edges on semiconductor surfaces: Application to Si/Si(001)

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A classical, hybrid Monte Carlo–molecular dynamic (MC-MD) algorithm is introduced for the study of phenomena like two-dimensional (2D) island stability or step-edge evolution on semiconductor surfaces. This method presents the advantages of working off lattice and utilizing bulk-fitted potentials. It is based on the introduction of collective moves, such as dimer jumps, in the MC algorithm. MD-driven local relaxations are considered as trial moves for the MC. The algorithm is applied to the analysis of 2D Si islands on Si(001). Results on early stages of island formation, island stability versus temperature and system size, and step-edge evolution are presented. In all cases good qualitative agreement with experimental results is found.

I. INTRODUCTION

The (001) surface of silicon is of utmost technological importance due to its wide range of applications in the micro- and optoelectronic industries. Moreover, it also provides an ideal model for the study of semiconductor epitaxy [1] as well as of a variety of surface structural modifications like reconstruction, island stabilization, and step-edge modification. Because of its relevance, a substantial amount of work has been done on this surface, yet several questions are still open. Among these are the determination of the equilibrium shapes [2] and thermal stability [3] of two-dimensional (2D) islands, or a precise description of step kinetics [4,5] or substrate modification in the presence of Ge or Si adsorbate [6].

The scarcity of definitive answers to these queries is related to the difficulty of carrying out thorough theoretical investigations. First, the use of large-scale simulations is necessary because experiments have shown that stable, or even long-lived, islands are constituted of at least several hundred atoms [3,7–9]. Similarly, Theis and Tromp [10] estimated a critical nucleus size of about 650 dimers. Simulating islands of such a size requires the use of systems whose surfaces are significantly larger than the islands themselves and of sufficient thickness that bulklike behavior is reproduced away from the surface. As can be easily seen, this means that at least several thousands of atoms are required for such a study. Second, it has been established that these processes occur on a time scale of the order of seconds [10–14], so that extended periods of time need to be simulated if these problems are to be addressed. Lastly, given that surface morphology, step kinetics, and island stability are temperature dependent [3,14–16], a realistic reproduction of nonzero temperature effects is also needed in the simulations.

Accurate *ab initio* methods are currently limited to systems composed of only a few hundred atoms at best. Tight-binding techniques can deal with bigger systems, but still in the range of a few thousand atoms. Both computational techniques have been successfully applied to the study of the Si(001) surface when focusing on problems like determination of the ground state reconstruction, analysis of absorption and diffusion sites, or identification of adatom diffusion paths. On the contrary, when attention is on the surface morphology, step kinetics, island stability, etc., classical methods are still preferable because of the need for large systems. Traditional classical Monte Carlo (MC) and molecular dynamics (MD) methods, while very effective in taking into account thermal effects, are too slow for simulating long-time-scale phenomena. In MD the need to integrate the equations of motion demands the use of time steps of the order of femtoseconds at best, so that millions of steps are necessary to cover a time span of a few nanoseconds. On the other hand, MC methods become inefficient in dealing with long-time-scale processes for which long-lived metastable states easily occur. As discussed in Sec. III A, this is exactly what happens when investigating surface modifications on the (2 × 1)-reconstructed Si(001). Kinetic Monte Carlo or standard MC using the solid-on-solid model have been successfully used when long-time-scale processes are involved [17–19], but they require a preknowledge of the possible diffusion mechanisms, and the simulation results are dependent on how well a large number of parameters is fitted. Moreover, the use of a solid-on-solid model forces discretization on the system, so that restrictions to the atomic motion are introduced.

In order to overcome the above mentioned problems related to dealing with long-time-scale processes, we have developed a classical hybrid Monte Carlo–molecular dynamics algorithm. The particular version presented here is targeted to the study of the Si(001) surface with Si or Ge adatoms, but the idea behind it is rather general and can be easily expanded to the study of other semiconductor surfaces. The main idea that this algorithm is based upon is to add the possibility of collective moves to the standard MC *single-atom* moves. With MC methods, the evolution of the system is definitely faster than with standard molecular dynamics; moreover, because of the collective moves, it is possible to overcome high potential barriers that otherwise would trap the system in metastable states. The identification of the collective moves to implement is the only point where knowl-

edge of the particular physical system under consideration is necessary. As an example, in the case of the Si(001) surface, the existence of a (2×1) reconstruction leads us to introduce the possibility of moving each dimer as a whole.

This paper is structured as follows. In Sec. II our method and general computational details are described. In Sec. III results obtained using only standard *single-atom* moves are shown first, then a detailed description of the implemented collective moves is presented, and, lastly, results obtained using this method are given. Conclusions are drawn in Sec. IV.

II. METHODOLOGY AND COMPUTATIONAL DETAILS

In this work, off-lattice constant-pressure Monte Carlo simulations [20] are used to study temperature-dependent structural properties of the Si/Si(001) surface. Simulations are performed in the canonical ensemble because, during each run, we want to keep both the number of particles and the temperature constant while bringing the system into equilibrium. The interatomic interactions are modeled using the classical Stillinger-Weber potential [21]. This potential has been chosen because several independent tests [22,23] found that it provides the best overall description of the Si(001) surface, especially at finite temperatures. Details of the parametrization can be found in Ref. [24]. Although classical potentials do not correctly reproduce dimer tilting (buckling) that occurs on the Si(001) surface [25,26], it does not represent a problem in this study because all the analyzed phenomena are driven by the coarse geometry of the system, in particular, by the presence of dimer rows, and this is well described in the model.

When not allowing collective moves, each MC step consists of two types of moves: small random displacements of individual particles and volume changes through the independent, random variation of each side of the simulation cell. The volume change is needed in order to keep the pressure constant at $P=0$. For each kind of move, including the collective one, acceptance probabilities are assessed using the standard METROPOLIS criterion.

As a simulation cell we use a slab geometry in which the unit cell is constructed along the [110], [1$\bar{1}$0], and [001] directions and periodic boundary conditions (PBC) are applied in the x and y directions only (z normal to the surface). The slab must be thick enough to have bulklike behavior in the center in order to guarantee independent evolution of the two surfaces and preparatory work showed that 24 atomic layers were sufficient for our purposes. Given that our primary interest is the study of surface phenomena, we have then always considered systems 24 layers thick and made the surface as large as possible. 22×22, 28×28, and 34×34 are typical surface sizes for which results are presented here. It must be noted, though, that in this paper we are mainly interested in exploring the algorithm capabilities, so we did not simulate extremely large systems. This means that the system sizes used during these simulations do not represent the largest systems treatable with this method.

Two kinds of phenomena are considered in this work: dimerization and step evolution/island stability. The details

of the (2×1) dimerization on the Si(001) surface are well known, so it can be used to test the capability of the potential and method together to reproduce the correct physics. Such an analysis is done utilizing two sets of simulations. First, we consider a silicon slab with (2×1)-reconstructed surfaces and a square island of Si on top of it. The island shows a (2×1) reconstruction in the direction perpendicular to that of the reconstruction on the surface. The aim of these simulations is to see if the (2×1) reconstruction on the surface disappears under the island. Second, we start from a silicon slab with the perfect diamond lattice structure, i.e., with unreconstructed (001) surfaces, and we let it evolve at constant temperature to see if it ends up with the correct (2×1) reconstruction. Typical temperatures considered are between 500 K and 1100 K when only single-atom moves are utilized and about 700 K when collective moves are included in the computation as well.

More complicated and perhaps more interesting simulations are performed with the purpose of studying step edges and island evolution. Experimentally, noticeable differences have been observed between terrace edges with dimerization parallel to the step edge (S_B or D_B) and those with dimerization perpendicular to it (S_A or D_A) [4,5], so that the investigation of the evolution of both edges appears to be an ideal application for our method. When investigating these problems, our initial system consists of a Si island on top of each slab surface. The surfaces are (2×1) reconstructed everywhere but under the island, which is square shaped and (2×1) reconstructed perpendicular to the surface reconstruction. The system evolves for some time after which configurations are analyzed. The standard duration for simulations like these is about 5×10^5 MC steps (MCSs) if only single-atom moves are used, while fewer than 10^5 MCSs are usually enough if coupled moves are considered as well. Typical temperatures are between 500 K and 900 K because of the interest in the temperature dependence of the physical quantities. By using square shaped islands as initial configurations we can follow the evolution of both S_A and S_B steps at the same time. Moreover, experimental results have shown that, before annealing, roughly squared islands are quite common on Si(001) surfaces [3,9,12]. For consistency between different simulations, we always began considering "nonbonded" S_B steps, i.e., steps that terminate on top of the underlying dimer rows.

As another application of our algorithm, we simulated the early stages of island formation. In this case we consider a (2×1)-reconstructed slab of silicon with randomly deposited dimers on it. The entire system then evolves at temperatures usually a bit higher than those used in the previously described simulations, so that events occur at a faster pace.

III. RESULTS

A. Single-atom moves only

In order to explain the need to include collective moves in the Monte Carlo simulations, we first present results obtained without them.

The simulations which were made to see if the (2×1) reconstruction on the surface disappears when an island is
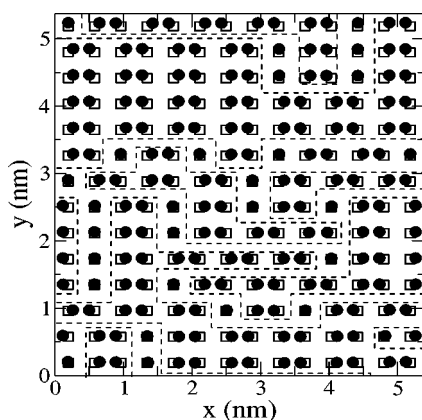
FIG. 1. Snapshot of a Si(001) surface at $T=580$ K. Open squares represent the initial positions and solid circles the positions after 10^6 MCSs. Dashed lines indicate antiphase domains walls.

deposited on top were always successful. On the contrary, we encountered several problems when trying to produce the (2×1) dimerization starting from unreconstructed surfaces. Figure 1 shows a configuration obtained after 10^6 MCSs at $T=580$ K as an example of what typically happens when we use only single-atom moves and begin with a completely unreconstructed surface. The open squares in the picture are the initial positions, corresponding to a perfect diamond lattice, and the solid circles are the positions after 10^6 MCSs. As expected, many dimers have formed, but the number of undimerized atoms greatly exceeds what is experimentally measured at similar temperatures. Moreover, unphysical antiphase domains have formed on the surface (shown in Fig. 1 by dashed lines). All these features do not improve with MC time: after a quick reorganization of the atoms at the beginning of the simulation, the configuration becomes almost frozen and only small oscillations of the atoms around their positions are observed. Both the excessive number of undimerized atoms and the antiphase domains are found in all simulations. They are, therefore, due to the method itself, and an immense number of MCSs would be required to see further changes.

It is known from *ab initio* calculations [27], and our results agree, that when two atoms with two dangling bonds each form a dimer, they lower their energy by about 2 eV/dimer. On the contrary, the energy gained when two or more dimers line up to form a dimer row is at least one order of magnitude smaller. This gain is actually so small that some classical potentials, e.g., that of Tersoff [22], find misaligned dimers to be energetically lower than dimer rows. In light of all this, the excessive number of undimerized atoms seen in our simulations can be easily explained. Early in the simulation the surface energy is significantly lowered when a dimer is formed, regardless of the resulting dimer alignment. Random formation of dimers obviously leads to a disordered surface, as shown in Fig. 1. Once this surface reorganization has taken place, the only way to eliminate "defects" (i.e., undimerized atoms) is to break existing dimers. In standard MC simulations the maximum displacement allowed to an atom in a single step is small compared to the interatomic distances, so that appreciable acceptance can be achieved.

Because of that, when only single-atom moves are considered, the removal of a defect requires first moving one atom in a dimer toward the defect, i.e., away from its neighbor. Later, the defect itself has to move close enough to its new neighbor to form a bond. During the first part of this process the original dimer is broken while the new dimer has not formed yet. The energy cost of breaking a dimer makes the first step extremely inconvenient energetically and results in an excessively low acceptance in a Metropolis MC simulation, since the acceptance probability depends exponentially on the energy difference between the initial and the final states. The reason for the formation of antiphase domains is similar. Once dimers have formed randomly on the surface, their rearrangement in organized rows can happen only via a series of intermediate configurations where one atom per dimer has moved away from its neighbor in order to align with a different dimer row. A state like this has high energy and is, therefore, extremely unlikely to be accepted.

Similarly unsatisfactory results were obtained when we tried to simulate the evolution of an island on top of the surface or adatom diffusion. In both cases the final configurations were practically identical to the initial ones, regardless of the length of the simulation. Again, this can be explained in terms of the energy cost of dimer breaking. If only small displacements are allowed for each trial move, it is extremely unlikely that an atom succeeds in moving away from a step edge or a nearest-neighbor (NN) surface atom because it would need to go through a series of energetically unfavorable configurations due to the inconvenient placing of its NN. On the other hand, if long jumps are allowed, one of the atoms forming a dimer may move away from its neighbor enough to break the dimer bond, and this, too, corresponds to a high-energy situation, i.e., to low acceptance.

B. Collective moves

1. Description

The simplest kind of collective move that we have considered is designed to aid the production of the (2×1) reconstruction when starting from an unreconstructed surface. This move includes what are henceforth referred to as *coupled jumps* and *row shifts* and turned out to be useful for a complete testing of the potentials [22].

When reviewing results obtained using single-atom moves only, we determined that the reason for the extremely low acceptance obtained once the dimers have formed was the high energy cost of the intermediate configurations. A natural solution to this problem is to introduce the possibility of moving two atoms at the same time (coupled jumps). This is accomplished by choosing an atom on the surface and randomly selecting its left or right neighbor along the direction perpendicular to the dimer rows. The two atoms are then randomly moved toward or apart from each other by a random amount, as shown in Fig. 2. In this way we rarely end up comparing a configuration with two dimerized atoms and an undimerized one to a configuration with three undimerized particles as always happens in the single-atom move case. Now, if a dimer is broken, another one is usually formed, so that the energy difference between the initial and
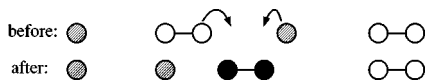
FIG. 2. Coupled jumps: dashed circles represent undimerized atoms, open circles are dimerized atoms, and solid circles indicate the new dimer that formed after the coupled jumps took place.

final configurations is rather small: consequently the acceptance is relatively high. This move is rather straightforward to implement, only requiring a larger cutoff for the Verlet list (list of neighbors) than that usually utilized for single-atom moves, because of the need for long jumps. Detailed balance is perfectly obeyed in this case. Similarly, we can speed up the elimination of the anti phase domains by introducing the possibility of shifting a row of dimers as a whole (row shifts). This is shown in Fig. 3. Using collective moves, all the simulations starting from unreconstructed surfaces ended up with the expected (2×1) reconstruction in a reasonably short computational time (about 6×10^4 MCSs).

The investigation of phenomena like edge evolution and island stability required the introduction of a different kind of collective move: the *dimer jump*, whose implementation is computationally more intensive. Here two atoms comprising a dimer undergo the same displacement (translation and small rotation) at the same time. To achieve significant modifications of the island edges in a relatively short time, we typically allow the particles to move up to 0.9 times the Si lattice constant $[a_0(\text{Si})]$) in the x or y direction in a single jump, while much less $[0.075a_0(\text{Si})]$ in the z direction. In some simulations we even used a maximum jump length of $1.4a_0(\text{Si})$. The amount and the direction of each jump are randomly chosen.

In Fig. 4 one example of atomic arrangement in the neighborhood of S_A and nonbonded S_B edges is shown. The open circles are the dimerized atoms on the surface, while the solid circles are the atoms in the island. Consider the S_B step: when any of the dimers from the island is moved along the negative y direction by any amount between 0.25 and 0.6 nm, it ends up in a position such that at least two of its nearest neighbors are too distant to effectively act as nearest neighbors. A similar problem is encountered at S_A and at rebonded S_B steps, with the difference that in the latter case the nearest-neighbor distances end up being too short. Summarizing, when considering a dimerized surface and a dimer jump as described above, the acceptance rate is really low because most of the time the post jump configuration ends up being extremely inconvenient energetically.

In order to achieve a much higher acceptance, once a dimer is displaced, we introduce the possibility of relaxing
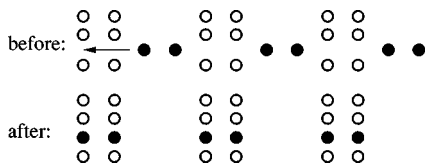

FIG. 3. Row shifts. Open circles represent dimers already aligned in rows; solid circles represent dimers out of alignment before the collective move.
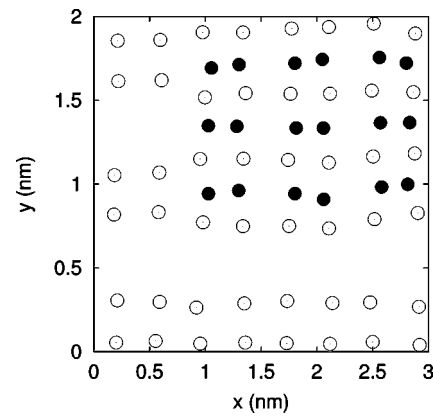

FIG. 4. Snapshot of part of an island after 5000 MC steps of relaxation at $T=700$ K (i.e., before dimer jumps are allowed). Open and solid circles are surface and island atoms, respectively. Parts of S_A and S_B steps are shown.

the local environment around it before deciding to accept or reject the move via the METROPOLIS algorithm (Fig. 5). As the *local environment* we consider all the dimer's neighbors before and after the move within a cutoff distance of $0.81a_0(\text{Si})$ and two layers from the surface. The dimer itself is included in such an assemblage as well. In Fig. 6 the local environment for one particular dimer is shown. The dimer (black spheres) is shown just after it has jumped, and at that time it only has two NNs. The local relaxation is performed using standard molecular dynamics with a velocity Verlet scheme for the integration of the equations of motion. Initial velocities are assigned from the Maxwell-Boltzmann velocity distribution at the simulation temperature, and constant temperature conditions are maintained using velocity rescaling. Test runs performed on different system sizes and under different initial conditions showed that, in most cases, a relaxation of seven MD steps using a time step of 10^{-15} s is enough for achieving a good acceptance rate.

Checking that detailed balance is obeyed is much more difficult in this case than when dealing with coupled jumps. We could not find a way to explicitly calculate the probabil-
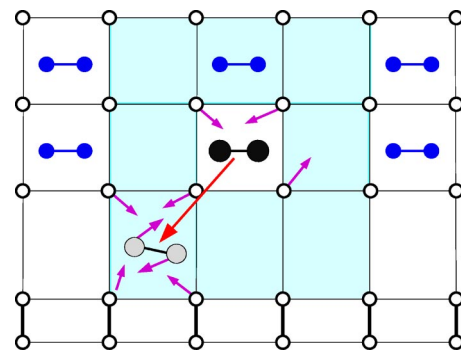

FIG. 5. (Color online) Dimer jumps: solid circles represent island atoms, open circles atoms on the surface. The dimer attempting to move is depicted by larger solid circles. The shaded area schematically indicates possible locations for such a dimer after the jump, and one example of "postjump" position is shown by the gray circles. The small arrows indicate possible displacement directions for the atoms that are allowed to move during the local relaxation.
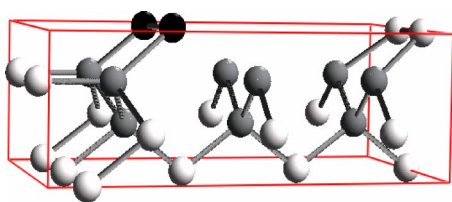
FIG. 6. (Color online) Dark gray spheres represent atoms that are moved during the local relaxation; light gray spheres represent some of their neighbors (for clarity not all of neighbors in the lowest layer are shown). The bonds are drawn for distances equal to or less than 2.715 Å. The dimer (black spheres) is shown just after it has jumped and, at this time, has only 2 NNs.

ity for the exact reverse path, once a dimer jump is accepted. However, no biases of any kind are applied when choosing the direction of the jump and the only effect of the MD loop is to relax the neighborhood of both sites where the dimer used to be and where it is as a result of the jump. On this basis we feel confident that no appreciable violation of detailed balance comes from the use of this collective move as long as the system is sufficiently relaxed before the dimer jumps are started. For the same reason, it is important that not too many moves are accepted during each MC step, so that enough time is given to the system to relax in between accepted dimer jumps. As a further test that possible detailed balance violation has no appreciable consequences on the evaluation of the physical quantities we performed a set of simulations where the local relaxation was done (less efficiently) using MC moves instead of MD. All the results of these simulations are qualitatively consistent with those obtained using MD relaxation, showing that the use of MD does not bias the system.

2. Results using single-atom and collective moves together

We first investigate the early stages of formation of two-dimensional Si islands on Si(001). This study was performed considering as initial system a slab of Si with (2×1)-reconstructed surfaces on top of which dimers are randomly deposited. Using the combination of single-atom and collective moves described in Sec. III B and the possibility of changing volume, the system is let to evolve at constant temperature. Temperatures typically used in simulations of this kind are around 900 K, because at this temperature enough events occur to allow the observation of the physical phenomenon within a reasonable number of MC steps: all our simulations reached equilibrium within a few hundred thousand MC steps.

A sample result is shown in Fig. 7: a snapshot of the (001) surface taken after 1.2×10^5 MSCs at a simulation temperature of 930 K. Solid circles are Si adatoms, while open circles represent surface atoms. The most noticeable feature is that most of the ad-dimers have combined to form almost monodimensional islands. This is consistent with what is observed experimentally [9,28]. Note that everywhere adatoms have come together the dimerization underneath has disappeared. A few transient configurations are still present: e.g., the one where three dimers have united and aligned parallel to the dimerization direction. This is not an indication of
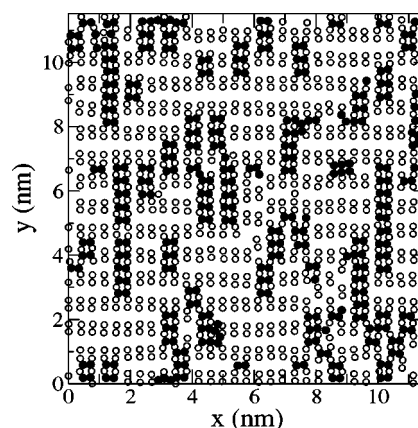

FIG. 7. Snapshot of Si over Si(001) after 1.2×10^5 MCSs for $T = 930$ K. Solid circles are adatoms; open circles are surface atoms. The surface contains 900 atoms (30×30, with PBC) and 170 dimers are deposited on top of it (the entire simulation slab contains 20 480 atoms).

unphysical behavior; it just means that the system has not yet reached complete equilibrium. Moreover, finding dimers in unexpected configurations emphasizes the fact that the dimer motion is not biased: they are allowed to rotate, to separate into undimerized atoms (as shown in Fig. 7 as well), and so on. All the results that we obtained studying the early phases of island formation are qualitatively identical to those presented here.

A second, independent problem we used to evaluate the applicability of our method is the study of island stability and step evolution. As described in more detail in Sec. II, we begin our simulations with a square island of Si over each Si(001) surface so that both S_A and S_B steps could be analyzed at the same time. Simulations are performed at different temperatures and using different system sizes, so that both thermal and size stability are tested. The kind of results we achieve is well exemplified by the instantaneous configurations displayed in Figs. 8–10. Comparing Figs. 8 and 9, it is easy to realize how well size stability is reproduced by our calculations: as experimentally observed [3,7,10], islands
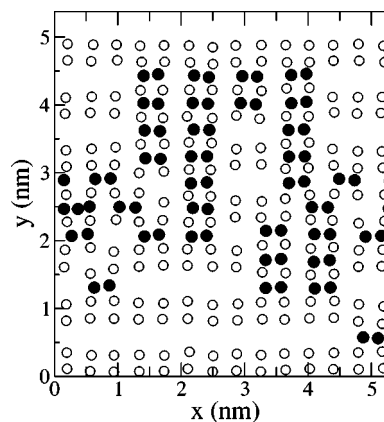

FIG. 8. Snapshot after 3×10^4 MCSs for $T = 700$ K. Solid circles are adatoms; open circles are surface atoms. The surface contains 196 atoms (14×14, with PBC) and the initial square island was made of 72 atoms.
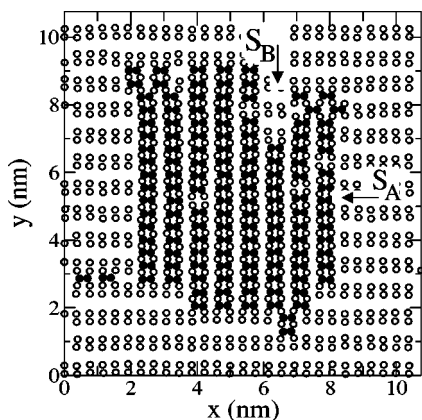
FIG. 9. Snapshot after 7×10^4 MCSs for $T = 700$ K. Solid circles are adatoms; open circles are surface atoms. The surface contains 784 atoms (28×28, with PBC) and the initial square island was made of 272 atoms.

smaller than a definite critical size are not stable even at relatively low temperatures. It is not the aim of this paper to accurately estimate such a critical size, but from these results it appears that our algorithm is suitable for such an inquiry.

From observation of Figs. 9 and 10, a dependence of the island stability on temperature can easily be inferred. In the two simulations the same system size was used, the only difference being temperature. After only 4000 MC steps the island that evolved at higher temperature (Fig. 10) is almost completely disordered, while the other is still very stable after 7×10^4 MCSs. This, too, agrees with previously reported experimental findings [3,12,15]. Analyzing Fig. 9 we note several other important features. First, S_A and S_B steps have evolved in a very different way: both the S_A steps are still significantly smooth, while the S_B steps have definitely become rough. The same behavior is consistently observed in scanning tunneling microscope images of terraces on Si(001) [4,8,14,29]. Second, the roughly square shape for the island has been preserved, in good agreement with experimental observations of silicon islands on Si(001) before annealing [3,9,12]. Lastly, dimer vacancies have appeared in
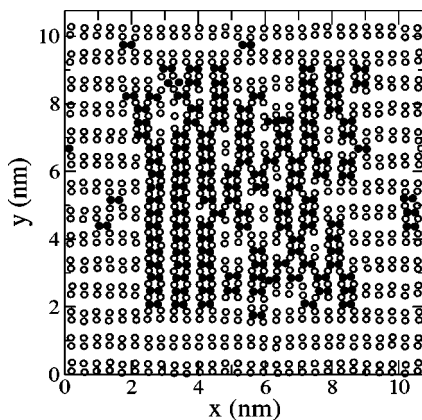

FIG. 10. Snapshot after only 4000 MC steps for $T = 928$ K. Solid circles are adatoms; open circles are surface atoms. The surface contains 784 atoms (28×28, with PBC) and the initial square island was made of 272 atoms.
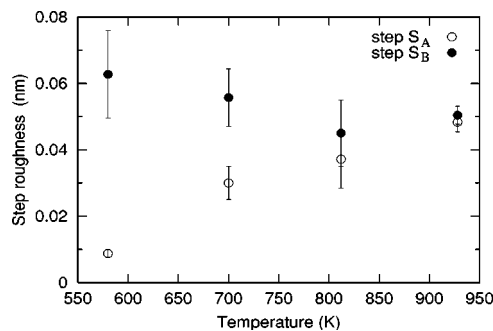

FIG. 11. Step-edge roughness vs temperature for islands initially square and composed of 272 (16×17) atoms (surface size $= 28 \times 28$ with PBC).

the island as the most widespread defect, and this, too, is a feature common to several experimental findings [3,9,12].

Finally, in order to show that this algorithm can also be used for quantitative evaluations of physical quantities, in Fig. 11 the step-edge roughness vs temperature is presented for a particular island size (16×17). The details of the computations are outlined elsewhere [30]. Again, a strong temperature dependence and a definitive difference in behavior between S_A and S_B steps is found as long as the islands are stable, i.e., for temperature below 900 K.

Similarly, a preliminary determination of the critical island size at $T = 700$ K ($k_B T = 0.06$ eV) is shown in Fig. 12(a). Islands initially containing fewer than 80 dimers have reduced their size by more than 25% before reaching equilibrium, indicating that they are not stable at this temperature. On the contrary, islands larger than 130 are stable at $T = 700$ K (their size at equilibrium is almost 90% of the initial one). In the case of islands initially made of 91 dimers, we observed fast island decays in some runs and great stability in others (for runs of about 1.5×10^5 MCSs, which justifies the larger error bar. An error bar almost as large is found for an initial size of 52, and is due to the fact that in some runs the island disintegration was not completed within the time length of the simulation. Corresponding results for step roughness and number of missing dimers are displayed in Figs. 12(b) and 12(c). As seen in experiments, the step roughness does not depend on system size and is higher for S_B steps than for S_A in the case of stable islands. The measure of the number of missing dimers per island (normalized on the initial island size) clearly shows a correlation between stability and the presence of defects, being definitely higher for stable islands (initial size lerger than 130 dimers) than for unstable ones.

IV. CONCLUSIONS

In this paper we have presented a hybrid MC-MD algorithm suitable for the study of large-scale, long-time-scale physical phenomena occurring on semiconductor surfaces. Compared to previously introduced methods, this has the advantages of being an off-lattice algorithm and of utilizing bulk-fitted potentials, i.e., not requiring additional
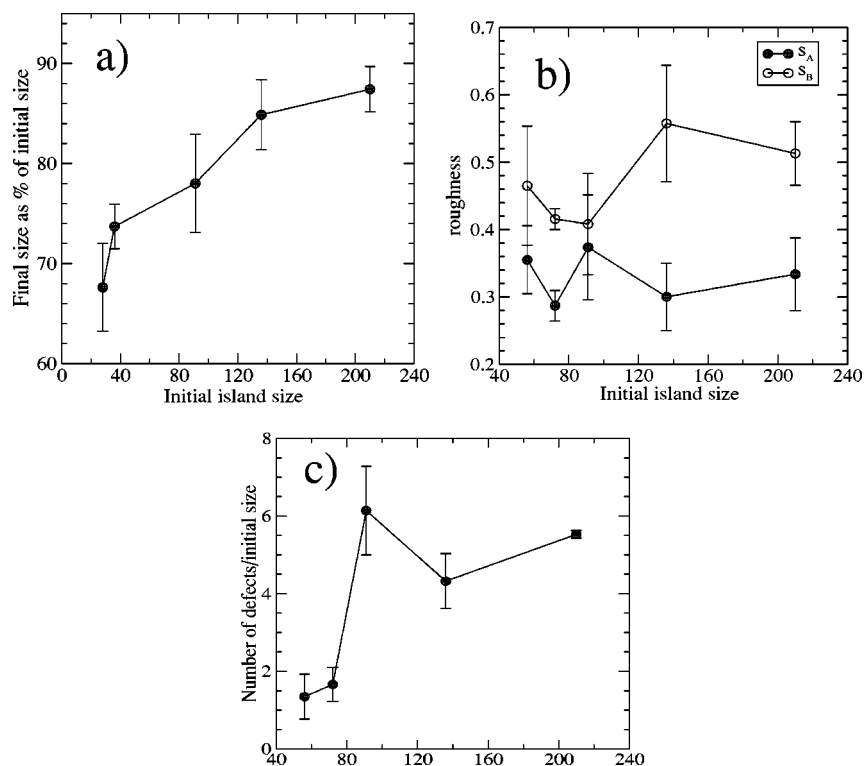
FIG. 12. Critical island size (a), step-edge roughness (b), and normalized number of missing dimers (c) vs initial island size at T $=700$ K ($k_B T = 0.06$ eV). All data are preliminary. The initial island size is always given as the number of dimers composing the island at time 0. In (a) the final size is given as a percent of the initial island size. In (b) and (c), data for islands below the critical size are taken before the disintegration starts.

parameters related to the surface phenomena under investigation. As an example, we applied it to the study of dimerization, step-edge evolution, and island stability on the Si(001) surface using the Stillinger-Weber potential. All the qualitative features attained as a result of our simulations are in good agreement with experimental results. Quantitative estimates of physical quantities can also be obtained using this method.

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