Effects of island disaggregation in growth models

K. Mazzitello,[1] C. M. Aldao,[2] and H. O. Mártin[1]

[1]*Physics Department, School of Exact and Natural Sciences, Universidad Nacional de Mar del Plata, Deán Funes 3350, B7602AYL Mar del Plata, Argentina*

[2]*Institute of Materials Science and Technology (INTEMA), Universidad Nacional de Mar del Plata-CONICET, Juan B. Justo 4302, B7608FDQ Mar del Plata, Argentina*

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We introduced two point island models with island disaggregation. In the first one, particles can detach from islands with an odd number of particles and from those with two particles. In the second model, particles can detach from all islands with more than two particles. The scaling exponents are analytically obtained and verified with Monte Carlo simulations. Specially, the power-law scalings of the island and monomer densities are analyzed. Comparison with other models indicates that the models introduced here present different scaling behaviors.

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I. INTRODUCTION

The growth of crystals by molecular beam epitaxy techniques has been studied with considerable attention for years [1–3] and continues to be a subject of interest [4–8]. The special case of the homoepitaxial growth of silicon on Si(100) has attracted a great deal of interest motivated by its technological applications [9,10]. Silicon atoms are deposited on a Si(100) surface at random with a constant flux. Deposited adatoms diffuse and nucleate when two of them meet forming dimers in a perpendicular direction to the substrate dimers. Chains of dimers are formed by the aggregation of new diffusing adatoms to dimers. A dimer *A*, a dimer chain *B*, and the corresponding growing sites are schematically shown in Fig. 1. Isolated dimers and dimer chains do not diffuse and will be generically named islands.

While at low temperatures all islands are stable, the detachment of particles from islands in the Si/Si(100) system takes place at sufficiently high temperatures. In typical experiments, at about 400 K a single adatom (particle *j* in Fig. 1) will detach if another adatom does not arrive (to site *i*) to form a new dimer within the residence time of the single adatom [11]. At this temperature, dimers are very stable [10], but at even higher temperatures the breaking of isolated dimers (as the island *A* in Fig. 1) becomes significant.

The effects of single particle detachment from islands has been recently studied in Ref. [12] using a point island model in a square lattice. In this model the detachment of particles is only allowed from islands with an odd number of particles (even islands do not break). These rules were motivated by the behavior of the Si/Si(100) system for which dimers and chain of dimers (i.e., islands having an even number of particles) are stable. In Ref. [12] it is shown that the scaling behavior of the model depends on the detachment probability.

In order to study the effects of dimer breaking in Si(100), in the present work we modified the above mentioned point island model allowing the breaking of islands with two particles. Since the growth of islands starts with the nucleation of two particles, we expected that single dimer breaking would have important consequences on the final surface morphology. Indeed, results show that dimer breaking is crucial in the growth scaling.

In previous models, islands with two particles can or cannot break, but the detachment of single particles can only occur from odd islands. In order to complete the study of the influence of the island breaking, we also analyze the case of particle detachment from all islands with more than two particles. This study corresponds to a simple model with magic clusters [13,14]. We found scaling behaviors of island and monomer densities as a function of coverage.

In a direct connection with the growth of dimer chains on Si(100), a dimer model with disaggregation of single particles from dimer chains and breaking of isolated dimers was also introduced. It was found that the behavior of this model is the same to that of the corresponding point island model.

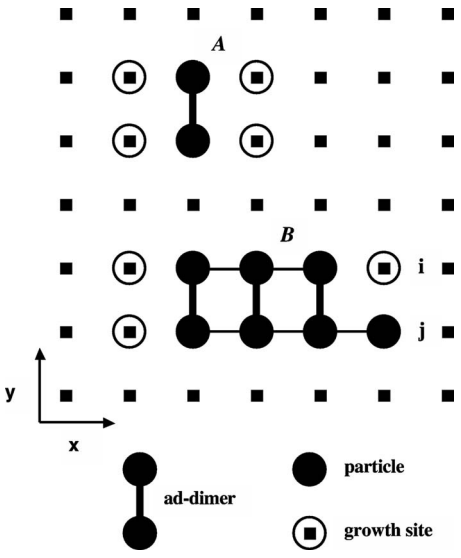

FIG. 1. The substrate (solid squares) and the growth of dimer chains. Two particles that become nearest neighbors in the *y* direction nucleate forming a dimer as shown in structure *A*. Next, particles can aggregate in growth sites to form a chainlike structure. Structures *A* and *B* correspond to an isolated dimer and to an island with an incomplete dimer, respectively.

II. MODELS

We will define three models, the dimer model and two point island models (model A and B). A square lattice of $L \times L$ sites represents the substrate, with $L=1000$, 3000. Periodic boundary conditions were used in order to avoid edge effects. We will assume that islands cannot diffuse and that the following processes take place: (a) deposition, (b) diffusion, (c) nucleation, (d) aggregation, and (e) detachment.

The rules for the dimer model are as follows.

(a) Deposition: each empty site of the lattice is occupied by a new particle with probability ε per unit time t.

(b) Diffusion: an isolated particle (i.e., a particle not bounded to an island) attempts to jump to any of its nearest neighboring (NN) sites with probability q per unit time. If the particle attempts to jump to an occupied site, the jump is not performed and the particle remains at its original position.

(c) Nucleation: if, as a consequence of diffusion or deposition, a particle arrives at an NN site in the y direction of a second isolated particle, these two particles always nucleate forming a dimer. This dimer plays the role of a seed for the dimer chain.

(d) Aggregation: Fig. 1 shows growth sites for different structures. If a diffusing or deposited particle arrives at a growth site, it always sticks, increasing the number of particles of the island by one.

(e) Detachment: each particle of an island, which does not belong to a dimer, can detach with probability p_1 per unit time (e.g., particle j of chain B in Fig. 1). One randomly selected particle of an isolated dimer can detach with probability p_2 per unit time (e.g., one particle of dimer A in Fig. 1). In both cases, the detached particle is placed on one of the NN sites of its original position selected at random, or remains in its original site if the selected NN site is occupied.

In the point island models, an island is composed of s particles ($s \geqslant 2$) that occupy a single lattice site. The rule of deposition for these models is the same as for the dimer model. Diffusion is also the same with the exception that if a particle attempts to jump to an occupied site by other particle, these two particles nucleate, forming a new point island with $s=2$ (this is the rule of nucleation). If the particle attempts to jump to an occupied site by a point island, it sticks, increasing the number of particles s of the island by one (i.e., $s \rightarrow s+1$, aggregation rule). Finally, the two point island models used in the present work differ in their detachment rules.

Model A: the detachment of particles from odd islands and from islands of size two (point dimers) is allowed. One particle of an island with an odd number of particles (i.e., $s \geqslant 3,5,\ldots$) can detach from this island with probability p_1 per unit time, and one particle of an island with $s=2$ can detach from this island with probability p_2 per unit time. The special case of $p_2=0$ was already studied in Ref. [12].

Model B: the detachment of particles from all islands with a size larger than two is allowed. A particle of an island with $s \geqslant 3$ can detach with probability p_3 per unit time. In both models the detached particle is shifted to one of the four NN sites of the island selected at random.

Simulations start with the lattice empty and run until the particle density θ (i.e., the mean value of particle per lattice site) reaches a desired value. We are interested in coverages low enough to avoid the percolation regime of extended island models [15]. Therefore, the used values of θ are below 0.15. For a fixed particle density, the dimer model and model A present four variable parameters, but it is expected that all processes depend only on the relative value of these parameters. Then, there are only three dimensionless independent control parameters, which we have chosen as $R=4q/\varepsilon$, $P_1=p_1/4q$, and $P_2=p_2/4q$. Similarly, for model B, $R=4q/\varepsilon$ and $P_3=p_3/4q$.

III. RESULTS

For point island models, let $n_s(t)$ be the density of islands (i.e., the average number of islands per lattice site) with s particles at time t. Note that $n_1(t)$ is the monomer density at time t. The total density of even islands N_E and odd islands N_O are given by

$$N_E = \sum_{s_{even}} n_s(t) \quad \text{and} \quad N_O = \sum_{s_{odd}} n_s(t), \tag{1}$$

where s_{even} (s_{odd}) runs over all even (odd) values of s, with $s \geqslant 2$ (i.e., $s_{even}=2,4,\ldots$, $s_{odd}=3,5,\ldots$). The total density of even islands with $s \geqslant 4$ will be denoted N'_E ($N'_E=N_E-n_2$). Finally, $N=N_E+N_O$ gives the total island density N. For the dimer model, the total island density (i.e., the average number of islands per lattice site) will be also denoted N.

Let us start presenting the results obtained with a model previously studied in which the detachment of particles from islands can occur [2,16]. In this case, islands with more than i particles are stable (i.e., they cannot break). For instance, for $i=1$ all islands are stable, for $i=2$ only islands with $s=2$ can break, and for $i=3$, only islands with $s=2,3$ can break. In the asymptotic regime ($R \rightarrow \infty$) the following behaviors have been obtained

$$N \sim R^{-\chi}, \tag{2}$$

$$n_1 \sim R^{-\omega}, \tag{3}$$

where $\chi=i/(i+2)$ and $\omega=2/(i+2)$ are the so-called island density and monomer density exponents, respectively.

We will now discuss model A. For $P_1=P_2=0$ there is no breaking of any island, and one recovers the well-known results $\chi=1/3$ and $\omega=2/3$, Eqs. (2) and (3) for $i=1$. For $P_1=0$ and $P_2>0$, only islands with two particles can break, and then $\chi=\omega=1/2$, Eqs. (2) and (3) for $i=2$. For $P_1>0$ and $P_2=0$, the disaggregation of only odd islands is allowed. As it was mentioned above, this case has been analyzed in Ref. [12]. For $R \gg 1$ and $P_1 \neq 0$ the main results obtained are

$$N \sim (P_1\theta)^{1/2}, \tag{4}$$

$$n_1 \sim P_1^{1/4} R^{-1/2} \theta^{-1/4}, \tag{5}$$

$$N_O \sim P_1^{-1/4} R^{-1/2} \theta^{1/4}, \tag{6}$$

$$N_E \cong N. \tag{7}$$

Then, when the dimensionless probability P_1 changes from $P_1=0$ to $P_1 \neq 0$ (with $P_2=0$), the island and monomer den-

sity exponents change from $\chi=1/3$ and $\omega=2/3$ to $\chi=0$ and $\omega=1/2$.

In Fig. 2(a) the Monte Carlo results of the island density N as a function of R for model A with different values of P_1 and P_2 are shown. It is found that $\chi=1/3$ for $P_1=P_2=0$, while $\chi=1/2$ for $P_1=0$ and $P_2>0$. For $P_1>0$ and $P_2=0$, and for large values of R, the island density reaches a constant value in agreement with Eq. (4). For $P_1>0$ and $P_2>0$ and large enough values of R, N behaves as $R^{-\chi}$, with $\chi=1/3$. Note that for $P_1=10^{-3}$ and $P_2=10^{-5}$, there is a crossover from $\chi=0$ to $\chi=1/3$, when R increases. Similarly, for $P_1=10^{-2}$, and $P_2=1$, a crossover from $\chi=1/2$ to $\chi=1/3$ is observed. For $P_1=P_2=0$ and for P_1, $P_2>0$, the same value of $\chi=1/3$ is obtained, but these cases correspond to different universality classes as it will be shown later. Similar behaviors were found for the dimer model as seen in Fig. 2(b). In short, for $P_1>0$, Monte Carlo results for both models strongly suggest that the island density exponent changes from $\chi=0$, for $P_2=0$, to $\chi=1/3$, for $P_2>0$, (including P_2 close to 0). In what follows, for the sake of simplicity, we will focus on the point island model A.

A. Model A. Disaggregation of dimers and islands having an odd number of particles

We can write rate equations by considering all possible processes that take place according to the rules for model A described above. The rate equation for the total island density N is

$$\frac{dN}{dt} = kn_1^2 - p_2 n_2 \tag{8}$$

where p_2 is the detaching probability from dimers, and k governs the monomer attachment rate. Dividing by ε, the particle deposition rate per empty site, we obtain

$$\frac{dN}{d\theta} = \frac{k}{\varepsilon} n_1^2 - P_2 R n_2, \tag{9}$$

where $d\theta=\varepsilon dt$ is the number of particles deposited per site during dt and we have considered that (see Sec. II)

$$\frac{p_2}{\varepsilon} = \frac{p_2}{4q}\frac{4q}{\varepsilon} = P_2 R. \tag{10}$$

For point islands $k \sim D$ [16], where D is the diffusion coefficient of monomers (in hops per unit time). In what follows we will consider that

$$\frac{k}{\varepsilon} \sim R. \tag{11}$$

When $R \gg 1$, a quasistationary regime exists in which $N \ll 1$ and $dN/d\theta \cong 0$ [17,18]. From Monte Carlo results it can be verified that $Rn_1^2 \gg 1$ in this regime. Then, from Eq. (9), we can write

$$n_1^2 \sim P_2 n_2. \tag{12}$$

The rate equation for the monomer density takes the form

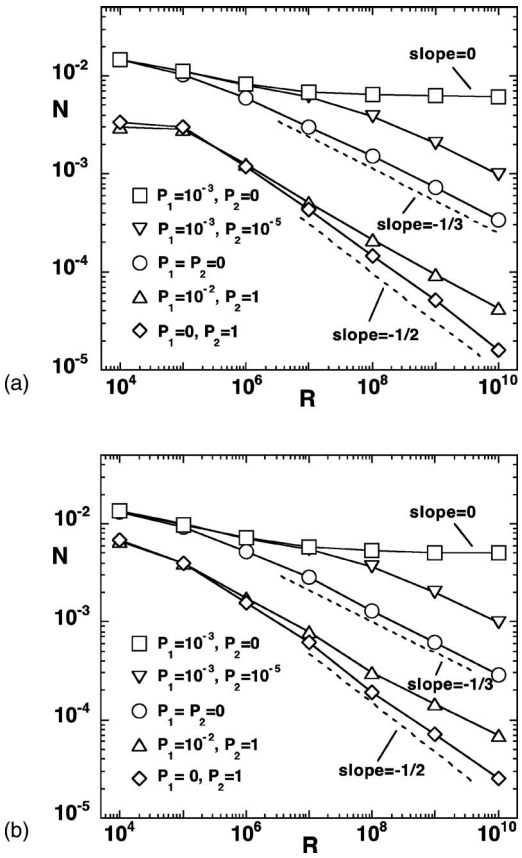

FIG. 2. The island density N against the parameter R, in a log-log plot, for different detachment probabilities P_1 and P_2, and $\theta=0.05$. (a) Corresponds to numerical results obtained from the point island model A and (b) from the dimer model. The same behavior is observed in both models.

$$\frac{dn_1}{dt} = \varepsilon - 2kn_1^2 + 2p_2 n_2 - kn_1 N + p_1 N_O, \tag{13}$$

where we have included the effects of deposition, nucleation, dimer breaking, aggregation, and detachment from odd islands. Dividing by ε we obtain

$$\frac{dn_1}{d\theta} = 1 - 2\frac{dN}{d\theta} - \frac{k}{\epsilon} n_1 N + P_1 R N_O, \tag{14}$$

where Eq. (8) and that $p_1/\varepsilon=P_1 R$ were taken into account. For $R \gg 1$, it is expected that $n_1 \ll 1$ and $dn_1/d\theta \cong 0$ [12,19]; then we can write

$$\frac{k}{\varepsilon} n_1 N - P_1 R N_O \cong 1. \tag{15}$$

It rests to analyze the rate equation for the density of odd islands

$$\frac{dN_O}{dt} = kn_1 N_E - kn_1 N_O - p_1 N_O, \tag{16}$$

where we have included aggregation to even and odd chains, and detachment from odd islands. Dividing by ε we obtain

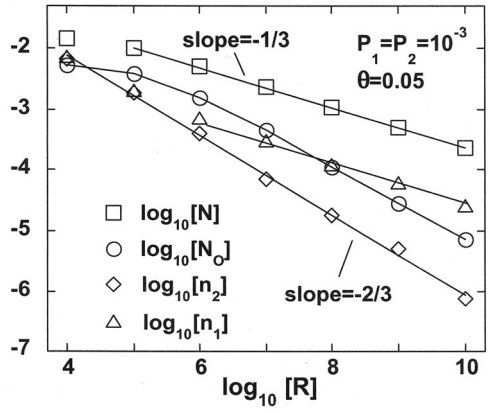

FIG. 3. The island density N, the monomer density n_1, the density of odd islands N_O, and the dimer density n_2 against the parameter R, in a log-log plot, for $P_1=P_2=10^{-3}$, with $\theta=0.05$ for model A.

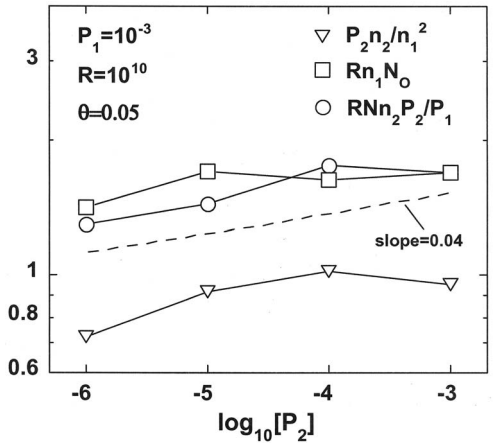

FIG. 4. The validity of Eqs. (22)–(24) is tested for $P_1=10^{-3}$, $R=10^{10}$, and $\theta=0.05$ (model A). Results were obtained averaging ten samples. A slope of 0.04 is shown as a guide to the eye.

$$\frac{dN_O}{d\theta} = \frac{k}{\varepsilon} n_1 N_E - \frac{k}{\varepsilon} n_1 N_O - P_1 R N_O, \tag{17}$$

that can be written as follows:

$$\frac{dN_O}{d\theta} = \frac{k}{\varepsilon} n_1 N - P_1 R N_O - 2\frac{k}{\varepsilon} n_1 N_O. \tag{18}$$

With Eq. (15), one obtains

$$\frac{dN_O}{d\theta} \cong 1 - 2\frac{k}{\varepsilon} n_1 N_O. \tag{19}$$

Since $dN_O/d\theta$ is small, it follows:

$$2\frac{k}{\varepsilon} n_1 N_O \cong 1. \tag{20}$$

Since the sum of the exponents for n_1 and N_O is -1, we expect the absolute value of the exponent of N_O to be smaller than 1. Thus, $P_1 R N_O$ must diverge with R as observed through numerical results. Equation (20) with Eqs. (12) and (15) yields

$$R n_2 N \sim \frac{P_1}{P_2}. \tag{21}$$

In short, from Eqs. (12), (20), and (21), the present analysis leads to the following relations among the relevant variables when $R \gg 1$:

$$\frac{n_1^2}{n_2} \sim P_2, \tag{22}$$

$$n_1 N_O \sim R^{-1}, \tag{23}$$

$$N n_2 \sim \frac{P_1}{R P_2}. \tag{24}$$

If $\chi=1/3$, as seen in Figs. 2 and 3, we can deduce that $\omega=1/3$ and that N_O and n_2 scale as $R^{-2/3}$. Indeed, in Fig. 3 this dependence is observed. Also, Eqs. (22)–(24) were tested over a wide range of values of R, P_1, P_2, and θ. In Fig. 4, it is shown that Eqs. (22)–(24) are valid in a wide range of P_2 values. Since $N=N_O+N'_E+n_2$, and N_O and n_2 scale as $R^{-2/3}$, $N'_E \cong N$ for $R \gg 1$.

B. Model B. Disaggregation of all islands except dimers

In model B all islands are unstable (particles can detach from islands) except the dimers. The density of unstable islands is given by

$$N_{uns} = \sum_{s>2} n_s(t). \tag{25}$$

Then, the rate equations for n_1, n_2, and N_{uns} are

$$\frac{dn_1}{dt} = \varepsilon - k n_1^2 - k n_1 N + p_3 N_{uns}, \tag{26}$$

$$\frac{dn_2}{dt} = k n_1^2 - k n_1 n_2 + p_3 n_3, \tag{27}$$

$$\frac{dN_{uns}}{dt} = k n_1 n_2 - p_3 n_3. \tag{28}$$

Summing Eqs. (27) and (28) and dividing by ε one obtains

$$\frac{dN}{d\theta} = \frac{k}{\varepsilon} n_1^2. \tag{29}$$

Equation (29) indicates that N grows irreversibly because of nucleation. An island is formed when two particles meet and will remain as an island, because the dimers do not break.

The solutions of these equations (for $R \gg 1$, $p_3/k \ll 1$, and low particle density) can be found as follows. When $R \gg 1$, a regime appears in which $n_1 \ll N$ and most islands will be dimers. Thus, we can write

$$N \cong \theta/2, \tag{30}$$

and then

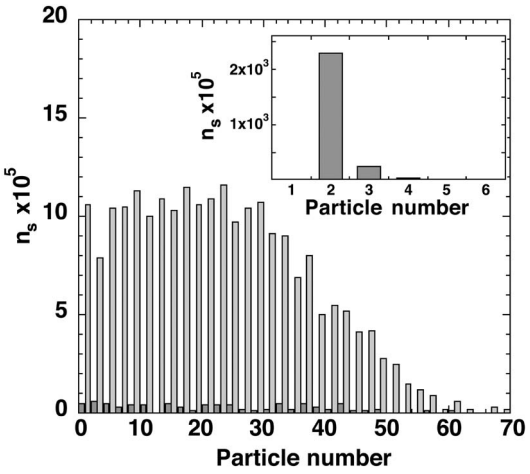

FIG. 5. Island density distributions versus particle number from numerical results obtained for the model with disaggregation of islands having an odd number of particles ($R=10^{10}$, $\theta=0.055$, $P_1=10^{-4}$, and $P_2=0$). The inset shows the island density distribution for the model with disaggregation of all islands except dimers ($R=10^{10}$, $\theta=0.05$, $P_3=10^{-4}$).

$$\frac{dN}{d\theta} \cong \frac{1}{2}. \tag{31}$$

Combining Eqs. (29) and (31), the dependence of n_1 with R can be deduced to be

$$n_1 \sim R^{-1/2}. \tag{32}$$

In Fig. 5 we present the island density distributions for a model in which disaggregation only occurs for islands having an odd number of particles and, in the inset, for a model in which disaggregation occurs in all islands except dimers (model B). In the first model it is clearly observed that most islands have an even number of particles and that islands with a large number of particles form. Conversely, in model B most islands are dimers and the monomer density is very small to be detected in the given scale.

From Eq. (26), considering that $dn_1/d\theta$ is very small, we can obtain the following:

$$N_{uns} \sim \frac{n_1 N}{P_3}, \tag{33}$$

and thus using Eqs. (30) and (32)

$$N_{uns} \sim \frac{\theta R^{-1/2}}{P_3}. \tag{34}$$

In Fig. 6(a) we present the dependence of N, n, and N_{uns} with R showing a good correspondence with the predicted results of Eqs. (31), (32), and (34). Also, Figs. 6(b) and 6(c) show the dependence with P_3 and coverage. As predicted, only N_{uns} depends on P_3 and N and N_{uns} directly depend on coverage.

IV. SUMMARY AND CONCLUSIONS

In order to study the effects of the disaggregation of islands we have shown two point island models. In model A

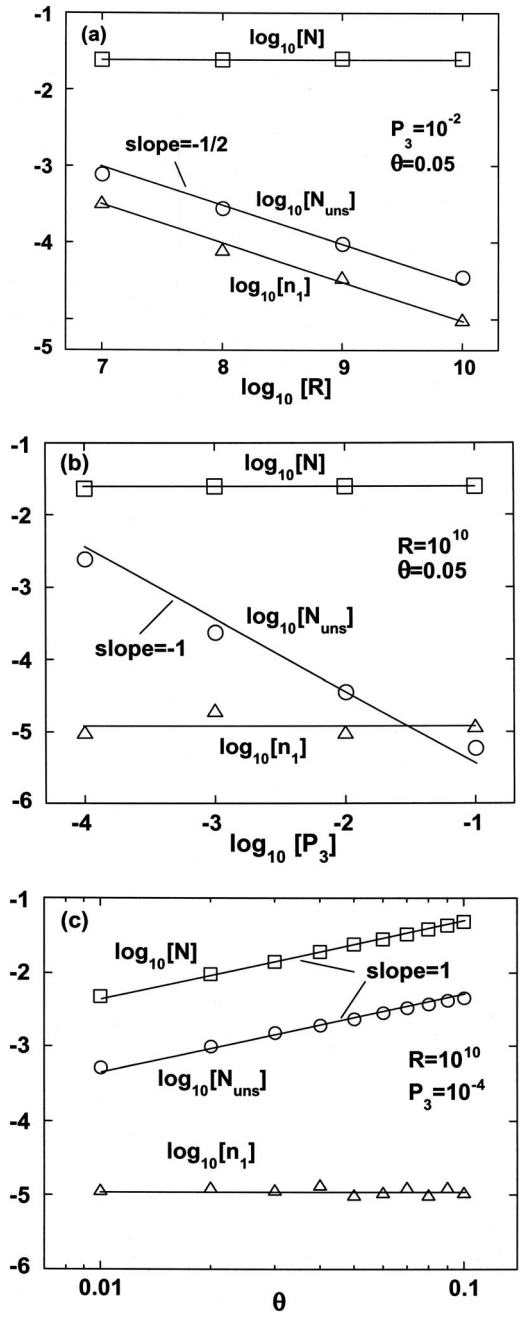

FIG. 6. The total island density N, the monomer density n_1, and the density of unstable islands N_{uns} against the parameter R (a), detachment probability P_3 (b), and coverage θ (c) for model B.

islands with an odd number of particles and with two particles can break with probabilities P_1 and P_2, respectively. In model B all islands with more than two particles break with probability P_3. The island density and monomer density exponents for both models are shown in Table I. The case of model A with $P_1>0$ and $P_2=0$ corresponds to a model (named C on Table I) previously studied in Ref. [12]. When $P_1=P_2=0$, the growth of the islands is irreversible and this case (named D) has been extensively studied (e.g., Refs. [2,16,17]). When $P_1=0$ and $P_2>0$ only point dimers can break and this case (named E) corresponds to $i=2$ in Eqs. (2) and (3). Finally, for the case in which all islands can break

TABLE I. Scaling exponents for models having different island disaggregation rules.

Model	Breaking of odd islands	Breaking of dimers	Breaking of even islands	Island density exponent χ	Monomer density exponent ω
A	Yes (with probability P_1)	Yes (with probability P_2)	No	1/3	1/3
B	Yes (with probability P_3)	No	Yes (with probability P_3)	0	1/2
C	Yes	No	No	0	1/2
D	No	No	No	1/3	2/3
E	No	Yes	No	1/2	1/2
F	Yes	Yes	Yes	1	0

(named F) $\chi=1$ and $\omega=0$, values that have been predicted as this corresponds to Eqs. (2) and (3) when i goes to infinity. From Table I, it can be seen that the model A presents a different scaling behavior. Comparing models A and C one concludes that the influence of dimer breaking is relevant. For instance, the island density exponent strongly changes when this breaking is allowed or not. This can be understood with the help of Eq. (8), the rate of island formation directly depends on two processes, the nucleation of particles and the breaking of point dimers.

Models B and C present the same N and n_1 exponents (see Table I). However, the behavior of the island density distributions as a function of the island size is quite different (see Fig. 5). In model B this distribution is dominated by n_2 since only dimers are stable. Furthermore, the behavior of N and n_1 as a function of θ for these models is different [see Eqs. (30), (32), (4), and (5)].

For small dimer chains (i.e., $\theta \leqslant 0.15$), numerical results obtained for the dimer model and for model A are qualitatively equivalent. Thus, the scaling laws given in Eqs. (22)–(24) are expected to be valid for the former case, where N_O corresponds to the island density of incomplete dimer chains.

While significant disagreements between the mean field predictions and the outcomes of Monte Carlo simulations and experiments on the exact island size distributions have been detected, the standard rate-equation approach has been successful in predicting the scaling behavior of average quantities such as the total cluster density [19–21]. The found discrepancy is due to the fact that the mean field approach ignores certain spatial correlations. The present work shows that in the introduced models, as in other models, the mean field approach and the Monte Carlo simulations agree regarding the scaling exponents.

In a recent paper [8], an interesting submonolayer growth model with disaggregation and mobility of islands was studied. In that model, the disaggregation rules do not take into account if islands have an even or an odd number of particles, that which has been specially addressed in the present work. Also, the detachment probability in the model of Ref. [8] depends on the island size, at odds with ours.

In summary, two point growth models, named A and B, in a square lattice with deposition, nucleation, aggregation, and detachment of particles have been shown and studied. Both models differ in their detachment rules (see Table I). The scaling behaviors for both models were analytically obtained and numerically verified. The scaling behaviors of models A and B and those corresponding to previously studied models mentioned in Table I are all different.

ACKNOWLEDGMENTS

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