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Side-branch growth in two-dimensional dendrites. II. Phase-field model

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The development of side-branching in solidifying dendrites in a regime of large values of the Peclet number is studied by means of a phase-field model. We have compared our numerical results with experiments of the preceding paper and we obtain good qualitative agreement. The growth rate of each side branch shows a power-law behavior from the early stages of its life. From their birth, branches which finally succeed in the competition process of side-branching development have a greater growth exponent than branches which are stopped. Coarsening of branches is entirely defined by their geometrical position relative to their dominant neighbors. The winner branches escape from the diffusive field of the main dendrite and become independent dendrites.

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I. INTRODUCTION

In the preceding paper [1] we presented experimental results on the growth of lateral branches in two-dimensional dendrites [2–12] both for small and large values of the Peclet number (large and moderate values of the diffusion length, respectively). For small Peclet number an almost self-affine fractal is observed. In this case and for short times a power law behavior is obtained for the growth of the branches before screening with exponents around 0.5 and 0.6. This initial stage turns out to be of crucial importance in the selection of the final pattern. Branches which are the largest at long times have the largest exponents and are the dominant from the initial regime. Apart from the initial stochastic disturbance, the growth process looks very deterministic and characterized by these exponents. The coarsening of branches is related to the competition process between neighboring branches and shows an exponential behavior. For large diffusion length the side-branches never become free dendrites but they remain prisioners of the lateral front of the main dendrite. Their velocities are not constant and they keep interacting by a screening-off process. Experimentally a hierarchy of sizes is obtained. For moderate diffusion length the faster branches escape from the diffusion field and become independent.

In this paper, we present a numerical study of the growth of branches with large Peclet number. To this purpose we use a phase-field model [12–22]. These models are based on the introduction of a set of partial differential equations for an order parameter coupled to a diffusive field. In this way we avoid the more complex treatment of integrodifferential equations to describe the interface. We use a standard phase-field model of solidification that has been validated extensively [14]. We are looking for a qualitative picture of side-branching and we corroborate the universal features obtained in experiments. We could interpret our results for moderate diffusion length in terms of the picture of large diffusion length of Ref. [1] with some differences. For example, in the initial stages the growth of branches is also described by a power law but the exponents are larger than in the case of large diffusion length. However, by increasing the diffusion length in the numerical calculations the values of the exponents are reduced. These results are in accordance with the experimental results in this regime. Regarding the screening-off effect, it is present in our numerical results for length scales smaller than the diffusion length. We observe that the slowest branches stop due to the screening effects of the larger neighbors and this effect is entirely dominated by geometrical reasons. For large time scales, we observe how the branches become independent of the main dendrite by accelerating and finally approaching the same constant velocity of the main dendrite in agreement with experimental results of Ref. [1] for large values of the Peclet number.

In Sec. II the phase-field model employed in this work is presented and the numerical procedure is discussed. In Sec. III we concentrate on the growth of individual side-branches. In Sec. IV the competition between side-branches and the screening-off process are considered. In Sec. V we present the results of the evolution of the winner branches for long times. The conclusions are given in Sec. VI.

II. MODEL AND NUMERICAL PROCEDURE

We have performed numerical simulations of the equations of a phase-field model for solidification [14,15,19,21]. The corresponding equations for the time evolution of the phase field $\phi(\mathbf{r},t)$, whose value varies between 0 (solid) and 1 (liquid), and the dimensionless diffusive field $u(\mathbf{r},t)$, whose value varies between −1 (supersaturated) and 0 (transition), can be written in the following form [21]:

$$\epsilon^2\tau(\theta)\frac{\partial\phi}{\partial t} = \phi(1-\phi)\left(\phi-\frac{1}{2}+30\epsilon\alpha\Delta u\phi(1-\phi)\right) - \epsilon^2\frac{\partial}{\partial x}\left[\eta(\theta)\eta'(\theta)\frac{\partial\phi}{\partial y}\right] + \epsilon^2\frac{\partial}{\partial y}\left[\eta(\theta)\eta'(\theta)\frac{\partial\phi}{\partial x}\right] + \epsilon^2\nabla[\eta^2(\theta)\nabla\phi], \qquad (2.1)$$

$$\frac{\partial u}{\partial t} + \frac{1}{\Delta}(30\phi^2 - 60\phi^3 + 30\phi^4)\frac{\partial \phi}{\partial t} = \nabla^2 u + \psi(x,y,t), \tag{2.2}$$

where lengths are scaled in some arbitrary reference length ω and times are scaled by ω^2/D, D being the diffusion coefficient. θ is the angle between the x axis and the gradient of the phase field and $\eta(\theta)=\sigma(\theta)/\sigma(0)$, $\sigma(\theta)$ being the surface energy. The characteristic parameters of this phase field [$\tau(\theta)$, Δ, α, and ϵ] are related to physical parameters. Δ is the dimensionless undercooling. The kinetic coefficient has been taken as isotropic (β_o), which leads to $\tau(\theta)=m\eta(\theta)$ with constant $m=c_pD\beta_o/Ld_o$, c_p being the specific heat per unit volume, L the latent heat per unit volume, and d_o the capillary length. α is equal to $\sqrt{2}\omega/12d_o$. The parameter ϵ controls the interface thickness and by $\epsilon\rightarrow 0$ the classical sharp-interface model is recovered. The term ψ introduces an external noise that induces side-branching [21].

The phase-field model equations have been solved on rectangular grids with mesh spacing Δx using first-order finite differences. In order to study dendrites we have considered a fourfold surface tension anisotropy $\sigma=\sigma(0)[1+\gamma\cos(4\theta)]$. The noise term is evaluated at each uncorrelated cell of lateral size Δx simply as Ir, where I denotes the amplitude of the noise, and r is a uniform random number in the interval $[-0.5, 0.5]$. We have used a set of parameters that gives rise to a needle without side-branching when $I=0$. The employed parameters are $\Delta=0.32$, $m=20$, $\alpha=400$, $\epsilon=0.006$, $\Delta x=0.02$, $\Delta t=2\times 10^{-4}$, $\gamma=0.1$, and $I=20$. The values of these parameters are chosen for numerical convenience. Our results may be grid and interface thickness dependent but our qualitative comparison with experiments does not depend on them.

III. GROWTH OF BRANCHES

First, we show in Fig. 1 a dendrite without side-branching obtained using the phase-field model with the set of parameters of Sec. II and taking $I=0$. The isoconcentration lines are indicated for different values ($u=-0.15$, -0.55, and -0.95). Two frames of reference are represented. The laboratory frame of reference $0X$, $0Y$ is chosen so that the dendrite grows along the $0X$ axis. The moving frame of reference $0X'$, $0Y'$ has its origin at the tip of the dendrite. We define the diffusion length $l_D(x)$ as the distance between the tip of the dendrite and the point of the isoconcentration line of value -0.95 that cuts the $0X$ axis. Moving further down the dendrite from the tip, the distance between the interface and the isoconcentration line for $u=-0.95$ is larger than $l_D(x)$. The gradient of the diffusion field in front of the tip is the largest in the dendrite, which makes the tip the fastest point of the dendrite.

Results presented in Ref. [23] give evidence of the two-dimensional character of dendrites studied in Ref. [1]. Thus the behavior of dendrites obtained in two-dimensional simulations is adequate to be compared with results presented in Ref. [1]. In Fig. 2 a dendrite with side-branching obtained by means of the phase-field model is presented at different times. The branches which are studied throughout this paper are labeled from 1 to 9. There is a competition process between branches at the scale of their lateral diffusion length. It can be observed that, at the time shown, branches 1, 4, 6, and 9 are winning their competition while branches 2, 3, 5, 7, and 8 seem to be affected by the diffusion field of their neighbors and thus screened.

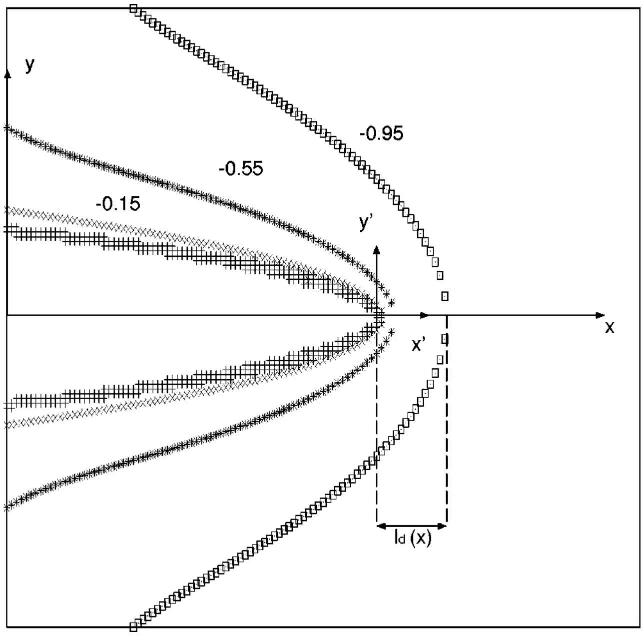

FIG. 1. Dendrite without side-branching obtained with the phase-field model. The isoconcentration lines of values -0.15, -0.55, and -0.95 are indicated.

Figure 3(a) shows the temporal evolution of the dendrite's tip position and the plot $y_n(t_n)$ of the growing length of six of the branches of the dendrite shown in Fig. 2, similarly to what we did in the experiment of the previous paper [1]. The temporal origin of y_n is taken when the tip of the dendrite crosses the point from which the protusion grows. It is shown that for the considered times, branches 2, 3, and 5 have already been screened and consequently they stop, while branches 1, 4, and 6 keep growing. The final state of the winner branches will depend on the interaction among them. If the lateral diffusion field is of the order of the distance between these branches, then another competition process is taking place. However, if the diffusion field is not

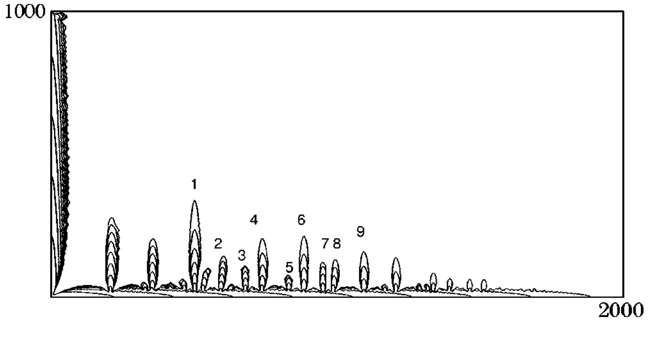

FIG. 2. Dendrite at different times obtained from the phase-field model. Considered branches are labeled from 1 to 9.

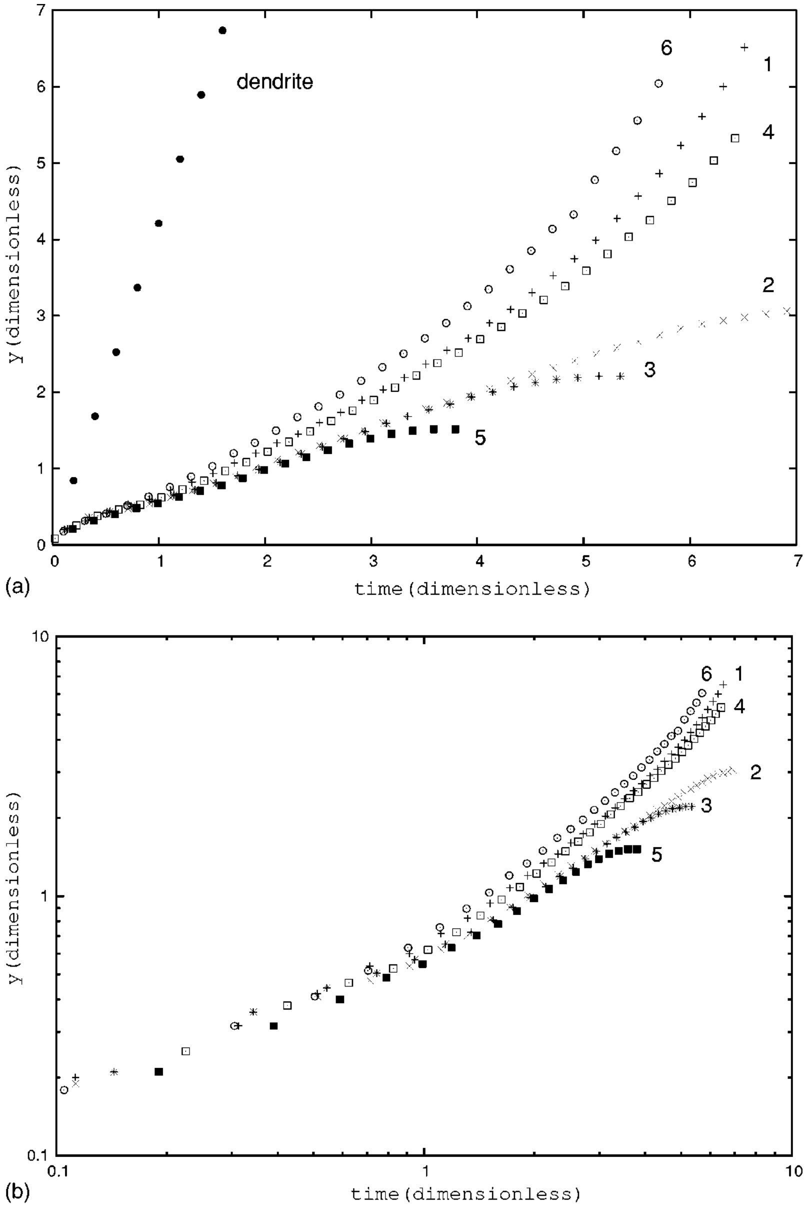

FIG. 3. (a) Dendrite's tip position and $y_n(t_n)$ for branches 1–6 as a function of time. (b) Log-log plot of $y_n(t_n)$ as a function of time for branches 1–6.

large enough, winner branches will finally behave as free dendrites, as it is explained in Sec. V.

In Fig. 3(b) we present a log-log plot of the data $y_n(t_n)$ of Fig. 3(a) where we confirm the power law growth of the branches described by the following equation:

$$y_n(t) = y_n^0 t_n^{\alpha_n}. \tag{3.1}$$

When fitting data obtained for different branches to Eq. (3.1), it is observed that winner branches grow from the initial stages of their lives faster than looser branches, which reveals an unexpected deterministic behavior in side-branching development. This conclusion is obtained systematically when comparing different branches. In Table I we present results for the value of the exponents α of branches 1–9. It has also been observed in our simulations that the value of the exponents decreases when the Peclet number is reduced. Thus the simulation results confirm the tendencies observed in Ref. [1].

TABLE I. Growth exponent α and screening parameters Y_o and S_o for branches 1–9.

Branch	α	Screened by	Y_o	S_o
1	0.68	not screened		
2	0.52	1 and 4	0.75	0.96
3	0.52	1 and 4	0.95	0.44
4	0.66	not screened		
5	0.61	4 and 6	0.86	0.55
6	0.67	not screened		
7	0.67	6 and 9	0.55	0.47
8	0.65	6 and 9	0.60	1.01
9	0.70	not screened		

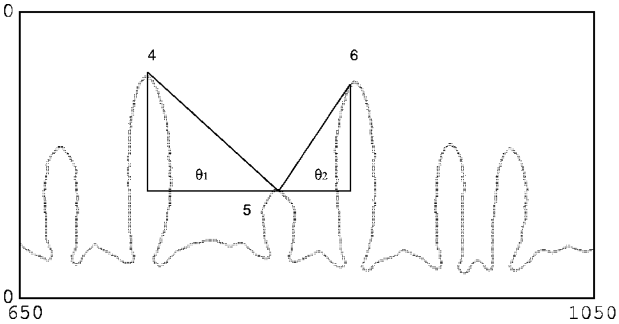

FIG. 4. Region of the dendrite containing different branches in competition. Branch 5 is being screened-off by branches 4 and 6. The angles of screening are indicated.

IV. COMPETITION BETWEEN BRANCHES: SCREENING-OFF PROCESSES

In this section we consider the competition between branches and the consequent screening-off effect in which some branches stop due to the close presence of faster neighbors. In Fig. 4 we present a region of the dendrite obtained by the phase-field numerical results where branches 4, 5, and 6 are in a competition process. The angles of screening of branch 5 are indicated. Although the birth of this branch was earlier in time than that of branch 6, this last one has a larger growth exponent and thus advances branch 5. At this moment, the screening-off effect of branch 6 on 5 adds to that of branch 4. Part of the solute diffused by both 4 and 6 concentrates in front of the tip of 5 and makes it stop.

The process of competition obtained in our simulations takes place under conditions of finite diffusion length, while in our previous paper [1] it was also shown the competition in an infinite diffusion length regime (i.e., a diffusion length of the order of the system size). In fact, for some considerations, we can consider a region such that containing branches 4, 5, and 6 as our whole system in a regime of infinite diffusion length. This means that the fact that we have a finite diffusion length only affects the large scales. For short lengths the screening-off effect could be described by a geometrical measurement. Following the procedure of the previous paper [1] we define a dimensionless quantity Y_n:

$$Y_n = (y_n^{Max} - y_n)/y_n^{Max} \tag{4.1}$$

where y_n^{Max} is the maximum length reached by branch n.

For any branch n screened by branches p and q, our geometrical measurement could be done by means of the screening angles θ_n^p and θ_n^q. We define the parameter S_n:

$$S_n = \tan\theta_n^p + \tan\theta_n^q \tag{4.2}$$

with $\tan\theta_n^p = (y_p - y_n)/(x_p - x_n)$ and $\tan\theta_n^q = (y_q - y_n)/(x_q - x_n)$.

We have studied the evolution with time of S_n for five different screened branches (labeled 2, 3, 5, 7, and 8 in Fig. 2) and an exponential relation between Y_n and S_n has always been found. We present in Fig. 5 a semilogarithmic plot of $Y_5(S_5)$ as described by the following equation:

$$Y_n = Y_0 \exp(-S_n/S_o). \tag{4.3}$$

In Table I we present the results of the fitting of Y_n for the considered screened branches. The results do not strongly depend on the diffusion length and are in excellent accordance with the experimental results of Ref. [1].

V. BEHAVIOR OF WINNER BRANCHES

In the previous section, we have studied the competition between branches. In this section we characterize the growth of the winner branches during their whole life, that is, birth, competition with neighbors, and final state as a free dendrite.

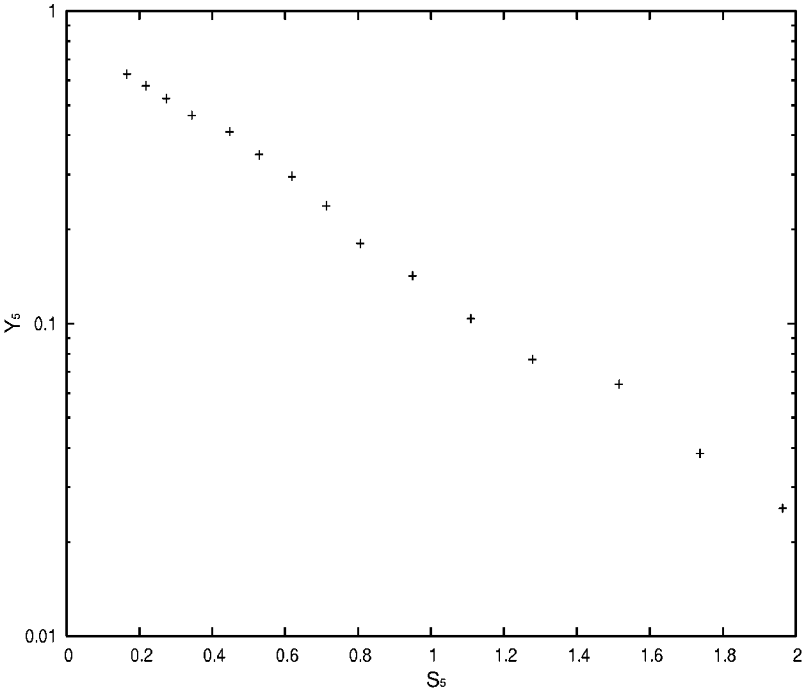

FIG. 5. Semilogarithmic plot of Y_5 as a function of S_5.

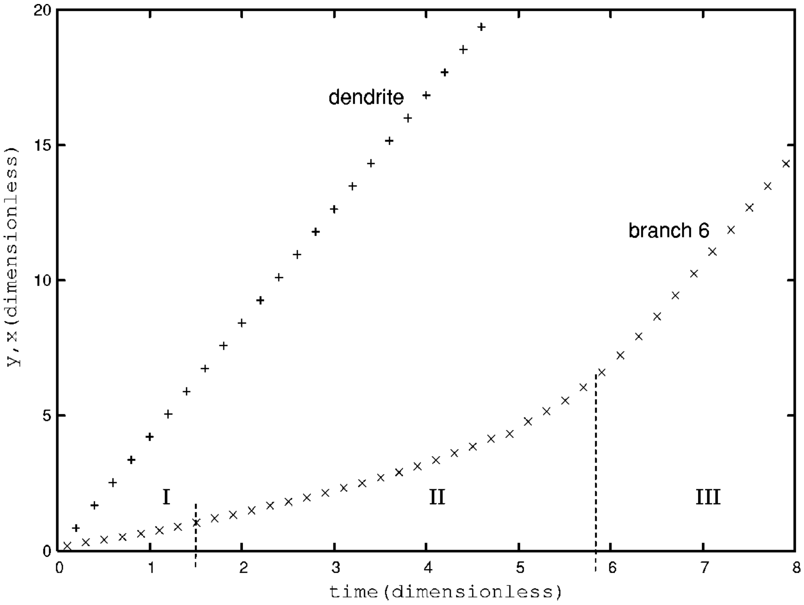

FIG. 6. Linear plot of the position x of the tip of the dendrite and the position y_6 of the tip of the winner branch 6 as a function of time.

As a difference with respect to the limit of infinite diffusion length, in the case of the finite value of l_d, the fast branches have the possibility to escape from the diffusion field front of the main dendrite. In Fig. 6 we present the temporal evolution of the position of the winner branch 6, y_6, and that of the tip of the dendrite x for long times. Three different regions in the behavior of branch 6 can be distinguished. For the initial times (region I) we observe a power-law growth as it was reported in Sec. III. In the second regime of intermediate times (region II) the branch has already won the competition process with its neighbors and accelerates. For large times (region III) the winner branch acquires the same constant value of the velocity of the main dendrite. Hence it finally behaves as a free dendrite. These three different behaviors have been observed in all the computed winner branches.

In Fig. 7 we show the temporal evolution of a disturbance (branch 6) that eventually becomes a free dendrite together with the isoconcentration line at $u=-0.95$. In Fig. 7(a) the small perturbation later associated to branch 6 does not affect the almost parabolic shape of the isoconcentration line (fluctuations observed in this line are associated to the noise induced in the simulations). In Fig. 7(b), the branch is already accelerating (time=9 in the simulation corresponds to time =4.5 after the birth of the branch, this is, region II in Fig. 6) and the isoconcentration line in front of it is already disturbed. In Fig. 7(c) branch 6 behaves already as a free dendrite (time=6.5 of Fig. 6, that is, region III) and it can be observed how the branch tends to perturb the isoconcentration line. In fact, the branch acquires its own concentration field, escaping from the global concentration field of the dendrite.

The competition process between branches makes the distance between the survivors λ increase with time. In principle one could expect that the increasing of λ took place until the moment in which the competition was finished and the winner branches grew as free dendrites. In Fig. 8 we present the results for the value of λ as a function of the diffusion length l_d associated to the tip velocity of the main dendrite at times in which considered branches behave as free dendrites. It can be observed that in general λ increases with l_d, although some points seem not to fully confirm this observation. This general tendency in the behavior of λ can be understood by considering that at larger values of l_d the diffusion field of winner branches reaches larger regions and thus the screening off affects a larger number of branches, which finally implies a larger distance between survivors. The discrepancy to this explanation showed by some points in Fig. 8 could come from the fact that once the competition process through the diffusion fields is over and winners grow as free dendrites, another process of interaction between branches can still take place. In fact, this process can always be present and consists in the stopping effect that secondary branches arising from a side branch can make on neighbor side-branches. During the whole process of dendritic growth and in particular when side-branches behave as free dendrites there are secondary branches which emerge from them that could eventually stop another free side branch by just growing in the region in front of it. In this case, this free growing side branch would not contribute to the measurement of λ and thus its value can be dramatically affected. Hence, although the plot of λ vs l_d gives information about the general behavior, it also shows that λ is probably not the most appropriate parameter to study dendrites in this regime of full development of side-branching. A set of alternative parameters could be the surface area and the contour length, whose behavior was analyzed in experiments [8,9], and numerically studied in Ref. [23].

VI. CONCLUSIONS

In this paper we have investigated the regime at large values of the Peclet number in a solidification process by means of a phase-field model. The growth of the individual side-branches is described by a power law at short times. The exponents become smaller for larger values of the diffusion length. At intermediate times an screening process is observed. At very large times winner branches accelerate. Ulti-

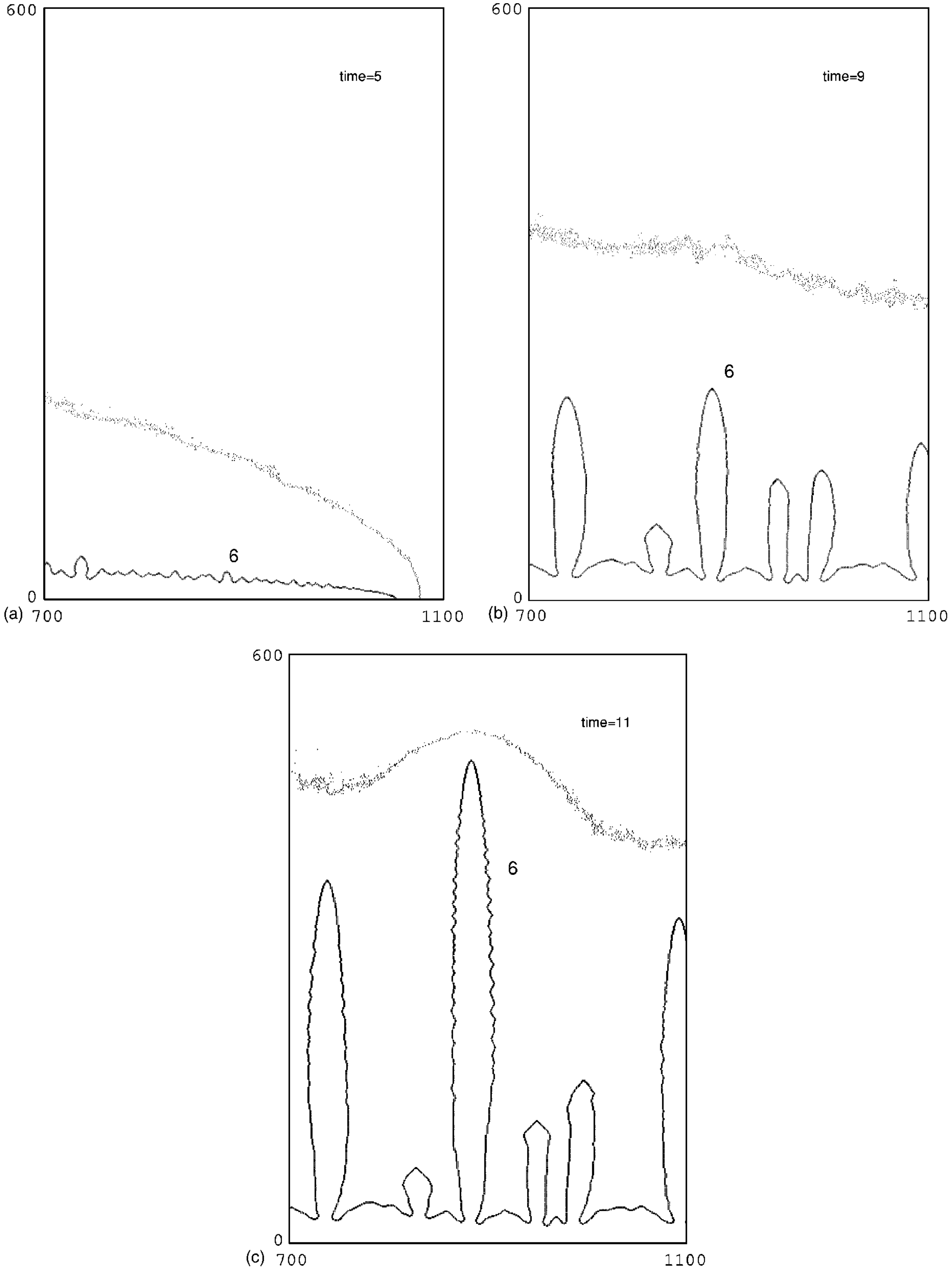

FIG. 7. Different plots of the temporal evolution of a disturbance that becomes a free dendrite and the isoconcentration lines at $u=-0.95$. (a) region I, (b) region II, and (c) region III.

mately they reach the velocity of the main dendrite and their velocity remains constant. These branches have escaped out of the initial diffusion front of the dendrite and have become independent dendrites. Our results corroborate qualitatively the picture of experiments which suggest that the noise mechanism plays a less important role in the determination of the final side-branching structure than expected. We have found that the competition process between branches is fully

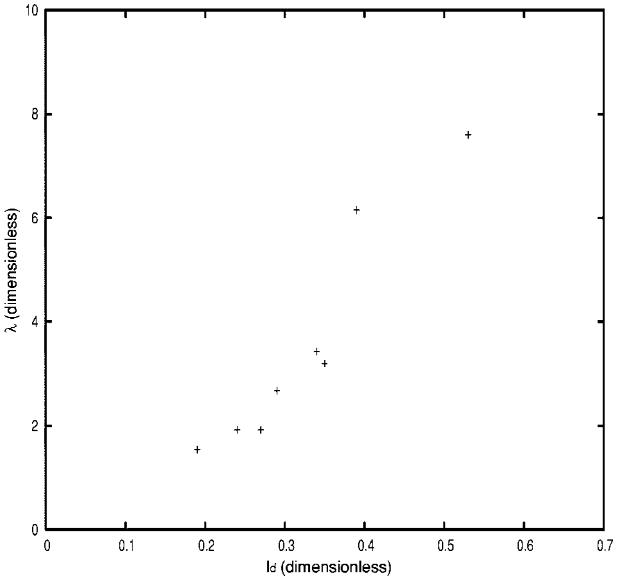

FIG. 8. Plot of the distance between freely growing branches as a function of the diffusion length associated to the tip velocity of the main dendrite.

determined from the beginning and the branch which starts growing faster succeeds. Our results may be grid and interface thickness dependent. A more quantitative comparison with experimental results would require a more accurate model such as the phase-field formulation with the thin-interface limit [16].

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