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Numerical illustrations to the paper "On mathematical modelling of growth of an individual crystal from melt in a non-uniform temperature field"

by

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The paper deals with numerical illustrations to the macroscopic model of the crystal growth, presented in L. Rubinstein (1983).

1. Introduction

In what follows we present several numerical illustrations to the model of the growth of a crystal in an inhomogeneous temperature field, as described in Rubinstein (1983). We recall that this model considers a lattice, representing "crystallits" and "virtual crystallits". The former and the latter are solid aggregates of macroscopic size, having a given crystallographic structure. It is supposed that the phase transition liquid → solid ($f \to s$) is a process of a spontaneous instant transfer of such a virtual crystallit C_f into a crystallit C_s. This process may occur when

1: The temperature of C_f is everywhere not greater than the thermodynamic equilibrium melting temperature T_m.

2: There exists within C_f at least one point where the temperature T is not greater than $T_m - \delta T_m$, with δT_m being a prescribed value of a minimal undercooling.

3: The amount of the latent heat to be released due to the transformation $C_f \to C_s$ is not less than the amount of heat needed for heating C_f from its temperature T up to the melting temperature T_m, plus the amount

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of heat which has to be accumulated for creating new phase interfaces minus the amount of heat which has to be released due to disappearance of existing phase interfaces.

4: The excess δq of the latent heat has to be instantly transferred into neighbouring crystallits/virtual crystallits which are not involved at the same moment into the phase transition $f \rightarrow s$ or $s \rightarrow f$.

Here we consider the simplest of possible cases where crystallits are thermally isotropic bodies whose thermal conductivity, heat capacity and density are constants coinciding with those of virtual crystallits. All those cells are squares with their boundaries parallel to boundaries of the region under consideration, where the prescribed temperature is maintained.

Our computations are performed for the abstract material whose physical properties are similar to those of Caesium. Namely we dual with the values:

$$\begin{gathered}\lambda = 0.054 \text{ cal/cm.sec.grad.}; \; c = 0.052 \text{ cal/g.grad.} \\ \varrho = 1.9 \text{ g/cm}^3; \; \gamma = 3.76 \text{ cal/g}; \; a^2 = \lambda/c\varrho = 0.445 \text{ cm}^2\text{/sec.} \\ T_m = 28.5^\circ\text{C}.\end{gathered} \tag{1}$$

Here $\lambda, c, \varrho, \gamma, a^2$ and T_m are, respectively, the coefficient of thermal conductivity, heat capacity, density, specific latent heat and the melting temperature. The value

$$\gamma_{sf} = -T d\sigma/dT \tag{2}$$

of the latent heat of creation of the interface solid-liquid may be chosen in such a way: The order of γ_{sf} is not greater than that of γ_{fv} — the latent heat of creation of the interface liquid — vapour, since the latent heat of melting is smaller than that of evaporation. The value of γ_{fv} may be roughly estimated by the use of the Eötvös constant K_E which is of order 2–3 $\text{erg/cm}^2 \geqslant$ grad (C.D. Hodgman, 1955). In our computations T is of the order 300°C. Hence γ_{sf} for our abstract body is definitely smaller than $10^3 \text{ erg/cm}^2 \cong 2.5 \geqslant 10^{-4} \text{ cal/cm}^2$. The maximal ratio of the length of new interfaces per one virtual crystallit to the area of the latter (we recall that we deal with a two-dimensional model) is no more than 4/H; we see that taking into account the latent heat γ_{sf} may appear to be significant only if H is small enough — for example H has to be of order 10^{-4} cm. Exceptionally by technical reasons connected with limitations for the use of the computer time, and with the only illustrative character of our computations we took the length of the crystallit boundary equal to 4H = .4 cm. Therefore in the most of computations we disregard the contribution of the latent heat of creation of new phase interfaces. However in one of the series of computations we deal not with physically reasonable values of γ_{sf} but with those enlarged up to 10^4 times. It is done in order to check the influence of the appearance of a "negative latent heat" in the approximation, connecting our model with classical Stefan problem, as described in Rubinstein (1983).

The presentation of the material is as follows. Section 2 is devoted to the description of the algorithm applied. Results of computations of illustrative examples, corresponding to the case of growth of an undercooled crystal, lying on the undercooled support and surrounded by an overheated melt are presented in section 3. Section 4 contains results of computations of the growth of a crystal surrounded by an undercooled melt, or in a partly undercooled and partly overheated melt. In the latter, quite incidentally chosen case, one may observe the appearance and growth of new crystals and their adjoining to the initially existing one. We are unable to qualify whether this observation is directly connected or not with the well known instabilities of free boundaries in the Stefan problem with a negative latent heat (Langer 1980; Ockendon, 1980). However such an example is seemingly worth of consideration. Results of the comparison of our and the classical Stefan approach are shown in section 5. Some discussion of the results obtained is offered in section 6.

2. The algorithm

We have no a priori information concerning the structure of the sequence

$$0 < t^1 < t^2 < t^3 < \ldots < t^n < \ldots \tag{3}$$

of moments of the spontaneous instant phase transition of any virtual crystallit/crystallit into crystallit/virtual crystallit within the region

$$G = \{x, y\colon -L < x, y < L\} \quad (L = 1) \tag{4}$$

under consideration. It is clear therefore that the algorithm to be proposed must include the discretization of the time axis with fine steps. Hence it seems natural to apply the explicit finite difference scheme. Let the region G be covered by the system

$$A = \{a_{km}\};\, a_{km} = (x, y\colon x_k < x < x_{k+1};\, y_m < y < y_{m+1}) \tag{5}$$

of crystallits/virtual crystallits. Here

$$x_k = kH;\, y_m = mH;\, H = L/N;\, k, m = 0, \pm 1, \pm 2, \ldots, \pm N \tag{6}$$

with the crystallit area equal to H^2. Assume, further, that every crystallit/virtual crystallit a_{km} is covered by a system of n^2 "mesh cells" b_{ij}^{km}:

$$b_{ij}^{km} = (x, y\colon x_{ki} < x < x_{k,i+1};\, y_{mj} < y < y_{m,j+1}) \tag{7}$$

with

$$x_{ki} = x_k + ih,\, i = 0, 1, \ldots, n-1;\, y_{mj} = y_m + jh;\, j = 0, 1, \ldots, n-1 \tag{8}$$

so that the area of every mesh-cell is equal to h^2.

Let now $\tau > 0$ be equal to the chosen time step and

$$t_k = k\tau;\ k = 0, 1, 2, \ldots \tag{9}$$

Denote by

$$t_{k_m} = t^m = k_m\,\tau;\ k_m < k_{m+1},\ m = 0, 1, \ldots \tag{10}$$

the sequence of all moments at which the phase transition of the type $c_f \leqslant c_s$ or $c_s \leqslant c_f$ takes place at least for one crystallit c_s or virtual crystallit c_f of the system A*).

Let us renumerate nodes of the above described network by setting

$$x_i = ih;\ y_j = jh;\ -nN \leqslant i, j \leqslant nN, \tag{11}$$

so that the cell a_{km} of the system A is now determined as

$$a_{km} = (x, y\colon x_{nk} \leqslant x \leqslant x_{n(k+1)};\ y_{nm} \leqslant y \leqslant y_{n(m+1)}),$$
$$k, m = -N, -N+1, \ldots, N-1. \tag{12}$$

Let

$$u_{ij}^k \cong \vartheta(x_i, y_j, t_k) \tag{13}$$

be the finite difference approximation for the temperature at nodes of our network. We must distinguish $\vartheta(x_i, y_j, t^m-0)$ and $\vartheta(x_i, y_j, t^m+0)$ since the instant change of the temperature due to the phase transition occurs at the moment t^m. Correspondingly we introduce notations

$$u_{ij}^{k_m-0} \cong \vartheta(x_i, y_j, t^m-0);\ u_{ij}^{k_m+0} \cong \vartheta(x_i, y_j, t^{k_m}+0). \tag{14}$$

Assume that $u_{ij}^{k_m-0}$ is determined for all $i, j\colon -nN \leqslant i, j \leqslant nN$. Denote by A_s^m the subset of A consisting of all virtual crystallits c_{ij}^f subject to the phase transition of the type $c_f \rightarrow c_s$ at the moment t^m+0. Let analogously A_f^m be the subset of A consisting of all crystallits c_{ij}^s involved at the moment t^m+0 into the phase transition $c_s \rightarrow c_f$. At least one of sets A_s^m or A_f^m is not empty. Let for the definiteness

$$a_{rp} \subset A_s^m. \tag{15}$$

Let, further, l_0 be the length of that part Γ_0 of the boundary Γ of a_{rp} along which a_{rp} is in a contact with those elements of A which are not involved into the phase transition at the moment t^m+0. Let δq_{rp}^m be equal to that excess of the latent heat released at $t = t^m+0$ within a_{rp} which has to be transferred at the moment t^m+0 through Γ_0 into adjacent cells. Denote

$$l_0/h = n_0. \tag{16}$$

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*) This means that $\exists a_{km} \subset A$ such that conditions 1–3, enumerated in the introduction are realized at least within one of the elements a_{km} of the system A for $t_{k_m-1} < t \leqslant t_{k_m}$. Hence the possible mistake in determining t^m is not greater than the length τ of one time step.

n_0 is equal to the number of mesh cells into which the instant heat influx occurs at $t = t^m + 0$. This instant heat influx implies the instant increase of the temperature of each of these mesh-cells of the value

$$\delta u_{rp}^m = q_{rp}^m / (n_0\, h^2\, c\varrho). \tag{17}$$

Let us now denote by ω_{rp}^m the whole set of mesh cells whose temperature instantly increases on the value δu_{rp}^m, and denote Ω^m the set of all ω_{rp}^m existing in G. Then

$$\begin{aligned} u_{ij}^{t^m+0} &= u_{ij}^{t^m-0} \quad \text{if } (x_i, j) \notin \Omega^m, \\ u_{ij}^{t^m+0} &= u_{ij}^{t^m-0} + \delta u_{rp}^m, \ \forall \omega_{rp}^m \subset \Omega^m. \end{aligned} \tag{18}$$

After determining $u_{ij}^{t^m+0}$, one may compute u_{ij}^k $\forall k \in (k_m, k_{m+1}-0)$ by the use of the boundary data and explicit scheme

$$\begin{gathered} u_{ij}^{k+1} = (a^2/h^2)\,(u_{i-1,j}^k + u_{i+1,j}^k + u_{i,j-1}^k + u_{i,j+1}^k) + (1/\tau - 4a^2/h^2)\, u_{ij}^k, \\ k = k_m, k_m+1, \ldots, k_{m+1}-0; \ -nN < i, j < nN. \end{gathered} \tag{19}$$

Evidently τ must be chosen according to the condition

$$\tau < h^2/4a^2 \tag{20}$$

of stability and be small enough in order to guarantee the desired accuracy of determining $\{t^m\}$.

3. The growth of a crystal lying on an undercooled support and surrounded by an overheated melt

Example 1

$$\vartheta(x, y, 0) = \begin{cases} 0.16 & (x, y) \in G_f, \\ -0.98 & (x, y) \in G_s, \end{cases} \tag{21}$$

$$\vartheta(x, y, t)|_\Gamma = \vartheta(x, y, 0)|_\Gamma \quad \forall t \geqslant 0. \tag{22}$$

Here

$$\begin{gathered} \Gamma = \bar{G} \backslash G;\ G = \{x, y{:}\ -1 < x, y < 1\}; \\ G_s = \{x, y{:}\ -0.1 < x < 0.2;\ -1 < y < -0.7\};\ G_f = G \backslash \bar{G}_s. \end{gathered} \tag{23}$$

Computations are performed for h = 0.025 and $\tau = 0.0003$ in two versions where the prescribed threshold of undercooling is equal to

a: $$T_m = 0.1 T_m, \tag{24$_\text{a}$}$$

b: $$\delta T_m = 0.1 T_m. \tag{24$_\text{b}$}$$

Results of computations are shown in Table 1 and in Fig. 1–3 where dimensionless x, y and t coincide numerically with dimensional values taken in CGS system*), and

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*) This relates to all the following computations.

Table 1

The sequence $\{t^m\}$ of the moments of phase transitions

Example 1

m		1	2	3	4	5	6	7	8
t^m	a	0.0087	0.0090	0.0213	0.0222	0.2625	0.2766	0.4008	0.4035
	b					0.2766	0.2781	1.3119	

m		9	10	11	The number of steps made after the last phase transition	
t^m	a	1.1022	1.2435	1.2660	10780	(The last phase transition at t^{11})
	b				10627	(The last phase transition at t^7)

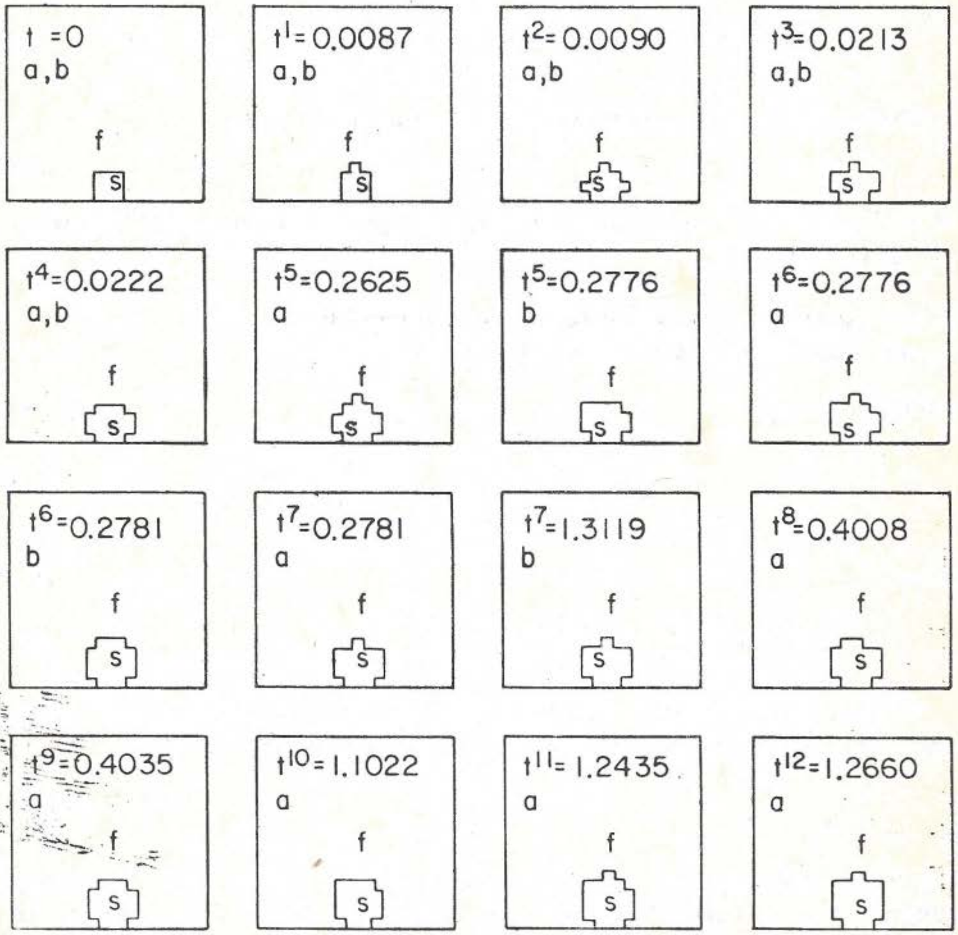

Fig. 1. The growth of a crystal located on the undercooled support. Example 1. a: $T_m = 0$; b: $\delta T_m / T_m = 0.1$

$$\vartheta(x, y, t) = (T(x, y, t) - T_m)/T_m \tag{25}$$

Graphs shown in Fig. 2, 3 illustrate the character of the temperature redistribution at moments of phase transitions. We see that at the moment $t = 0.0087$ there is the transition of one virtual crystallit into crystallit, whereas at the moment $t = 0.0213$ two virtual crystallits are transformed into crystallits. Fig. 1 contains a sample of the crystal shape and location.

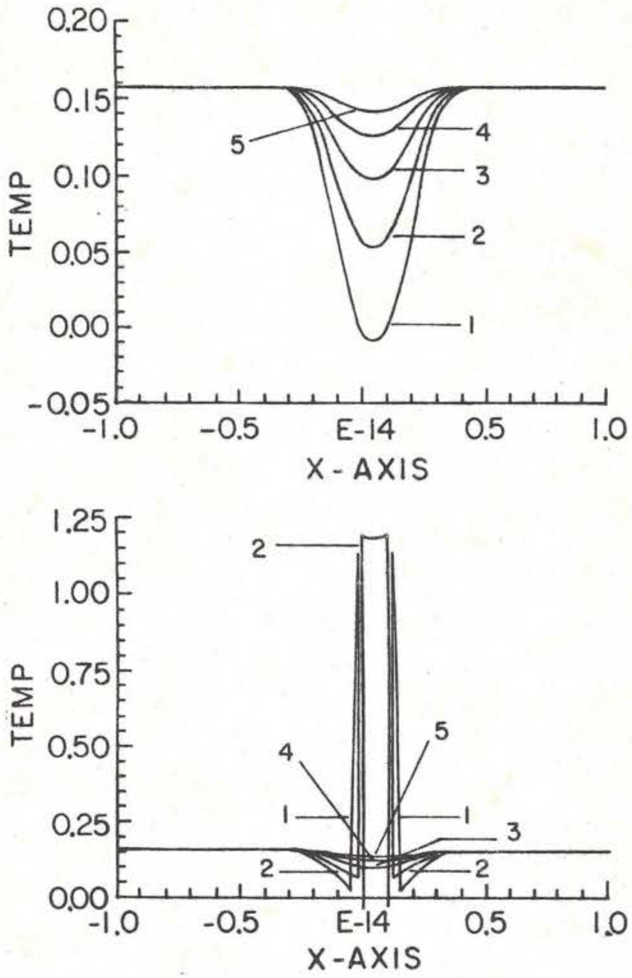

Fig. 2. The growth of a crystal located on the undercooled support. Example 1. The temperature distribution. a: $t = 0.0087-0$; b $= 0.0087+0$; $\delta T_m/T_m = 0.1$; 1: $y = 0.500$; 2: $y = 0.525$; 3: $y = 0.550$; 4: $y = 0.575$; 5: $y = 0.600$

The great speed of the process is stimulated by the great degree of undercooling of the support on which the crystal lies. Such a great undercooling is chosen in order to reduce the duration of computations. It evidently is agreeable because of the only illustrative character of our computations.

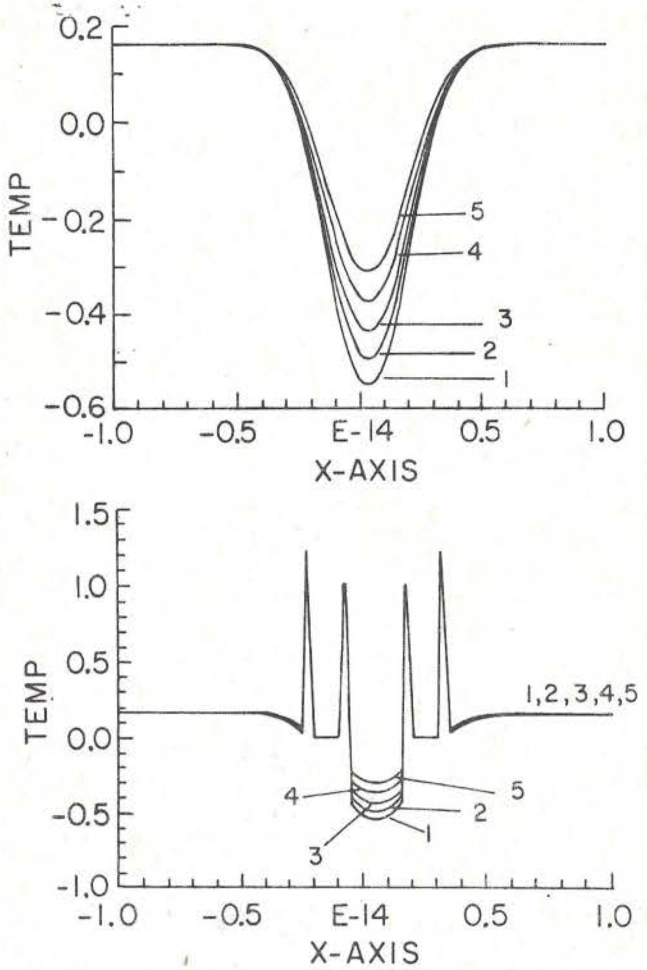

Fig. 3. The growth of a crystal located on the undercoöled support. Example 1. The temperature distribution. a: $t = 0.0213-0$ b: $t = 0.0213+0$; $\delta T_m/T_m = 0.1$; 1: $y = 0.300$; 2: $y = 0.325$; 3: $y = 0.350$; 4: $y = 0.375$; 5: $y = 0.400$

Initial and boundary conditions of the example under consideration are almost symmetric and uniform in each of the phases. The minor asymmetry of the initial location of a growing crystal implies only small asymmetry which completely disappears at the moment of the last phase transition in both cases a and b. In order to deal with the strongly asymmetric and inhomogeneous case, the example 2 is considered.

Example 2. The distribution of the boundary temperature and the location of the crystal at the initial moment are shown in Fig. 4. The initial temperature is taken equal to

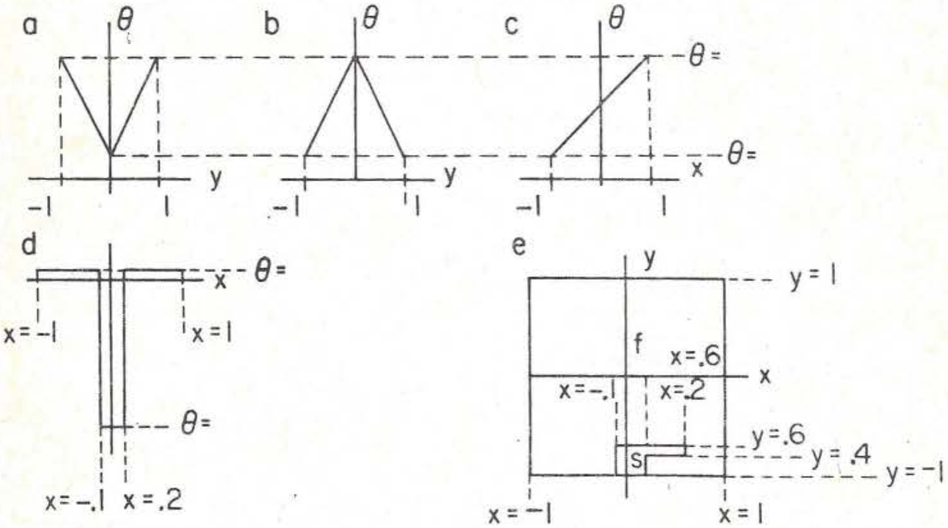

Fig. 4. The growth of a crystal located on the undercooled support. Example 2. The input data

Table 2

The sequence $\{t^m\}$ of the moments of phase transitions

Example 2

m		1	2	3	4	5	6	7	8
t^m	a	0.0021	0.0024	0.0030	0.0075	0.0093	0.0096	0.0099	0.0102
	b	0.0021	0.0024	0.0030	0.0075	0.0093	0.0096	0.0099	0.0102
m		9	10	11	12	13	14	15	16
t^m	a	0.0120	0.0123	0.0189	0.0219	0.0222	0.0225	0.0237	0.0246
	b	0.0120	0.0123	0.0189	0.0342	0.0345	0.0354	0.0393	0.0465
m		17	18	19	20	21	22	23	24
t^m	a	0.0279	0.0288	0.0300	0.0324	0.0336	0.0375	0.0381	0.0414
	b	0.0624	0.0960						
m		25	26	27	28	29	30	31	32
t^m	a	0.0417	0.0441	0.0447	0.0516	0.0531	0.0540	0.0567	0.0639
m		33	34	35	36	37	38	39	40
t^m	a	0.0693	0.0699	0.0711	0.0747	0.0810	0.0849	0.0942	0.1089
m		41	42	43	44				
t^m	a	0.1125	0.1197	0.1266	0.1479				
The number n of steps performed after the last phase transition of the number m			m	a b	44 18	n	a b	14507 14680	$\tau = 0.0003$

$$\vartheta(x,y,0)=\begin{cases}0.02 & \text{in } G_f,\\ -0.98 & \text{in } G_s.\end{cases} \tag{26}$$

The sequence of moments of the phase transitions in both cases a and b (see (24_a) and (24_b)) is presented in Table 2.

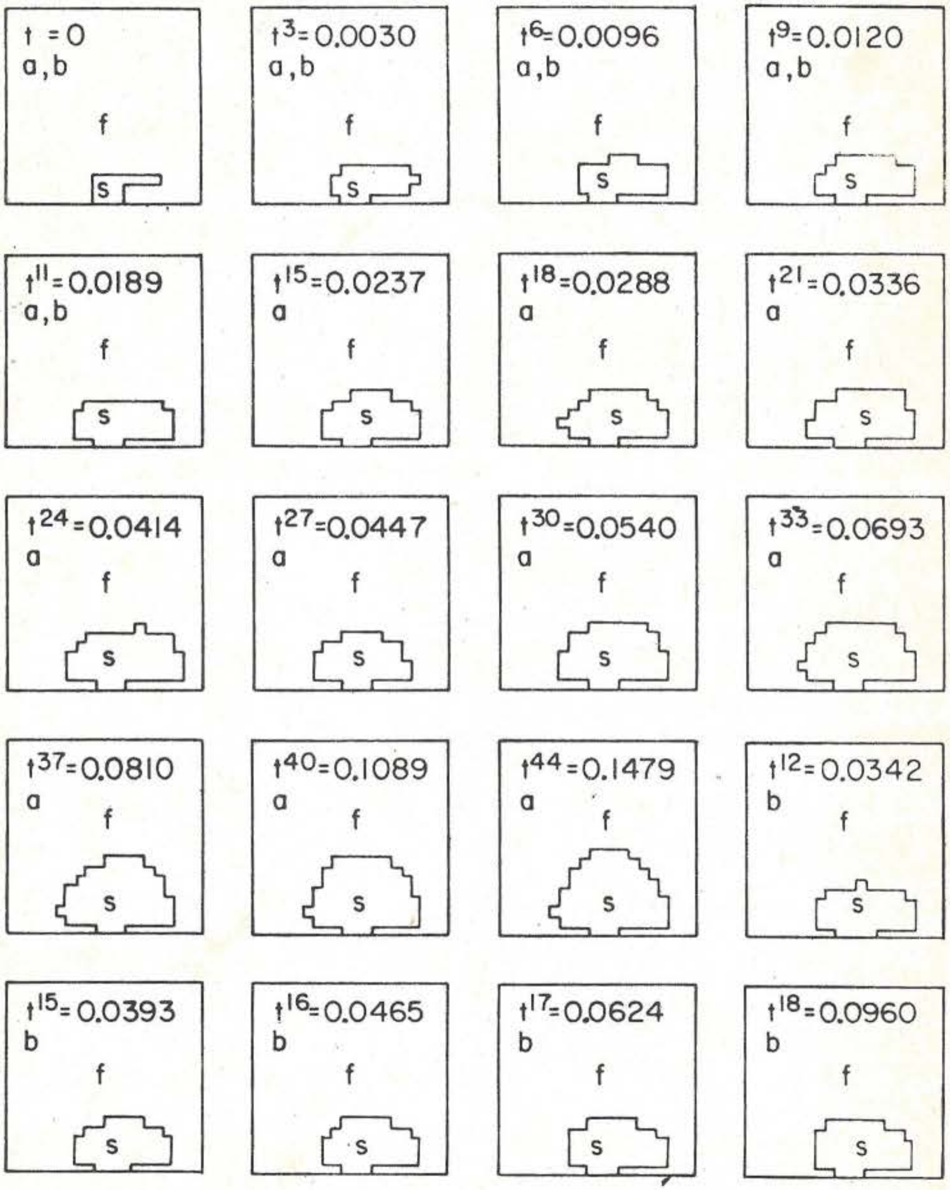

Fig. 5. The growth of a crystal located on the undercooled support. Example 2. a: $\delta T_m = 0$; b: $\delta T_m/T_m = 0.1$

The character of the respective crystal growth is shown in Fig. 5. It is seen from Table 2 and Fig. 5 that the frequency of phase transitions and the "final" crystal shape are strongly affected by the value of the threshold of undercooling. The same takes place in example 1 but in a less appreciable degree.

4. The growth of a crystal immersed into a partly undercooled, partly overheated melt

The model under considereation is described in Rubinstein (1983) for a crystal located on an undercooled support and surrounded by a melt with the bulk temperature greater than that of melting. However it may be also used for description of the growth of a crystal immersed into a undercooled melt. In the traditional approach (Langer, 1980) it is always supposed that there exists only one growing crystal whose temperature is identically equal to that of melting. This means that the appearance of new crystals is considered as impossible and this prohibition excludes the necessity of dealing with the coalescence of small crystalls (clusters) with the initially existing one. We also recall that this kind of the treatment of the process of solidification leads to the necessity of considering a specific problem of the phase-interface instability (Langer, 1980; Ockendon, 1980). This problem arises when one does not take into account the impact of the surface tension onto the melting temperature. If the influence of the surface tensions is taken into account, the phase interface in the classical Stefan problem appears to be stable. In our model no specific stability problem arises. Indeed, the temperature distribution between every two moments of phase transition is subordinated to the homogeneous heat conduction equation which has to be valid within both phases, belonging in such a time interval to the fixed regions*).

We have considered two cases: 1) The crystal at the melting temperature is immersed into a completely undercooled melt and 2) the melt, into which the crystal at the melting temperature is immersed, is partly undercooled and partly overheated. In the first of these two cases we observe extremely rapid solidification of the whole region, which is the result of the greatness of the undercooling imposed on the system. Rather more impressive picture is obtained in the second case the description of which follows.

Example 3. Let us divide the region G into 9 subregions:

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*) This relates to the general case where the heat capacity, thermal conductivity and density of solid phase differ from those of the liquid phase. In our simplified case the heat conduction equation has to be valid within the whole region G $\forall t\ (t^m, t^{m+1})$; $m = 0, 1, 2, \ldots,$ $(t^0 = 0)$.

$$\begin{aligned}
G_1 &= \{x, y\colon -L< x, y < -l\};\\
G_2 &= \{x, y\colon -l < x < l;\ -L< y < -l\};\\
G_3 &= \{x, y\colon l < x < L;\ -L< y < -l\};\\
G_4 &= \{x, y\colon -L< x < -l;\ -l < y < l\};\\
G_5 &= \{x, y\colon -l < x, y < l\};\\
G_6 &= \{x, y\colon l < x < L;\ -l < y < l\};\\
G_7 &= \{x, y\colon -L< x < -l;\ l < y < L\};\\
G_8 &= \{x, y\colon -l < x < l;\ l < y < L\};\\
G_9 &= \{x, y\colon l < x, y < L\}.
\end{aligned} \tag{27}$$

Define the initial temperature by the equalities:

$$\vartheta(x,y,0) = \begin{cases}
2\sin\left(\frac{1}{4}\pi(x+y-2L+4l)/(L-l)\right)\sin\left(\frac{1}{4}\pi(x-y)/(L-l)\right) & \text{in } G_1\\
\sin(\pi|x|/l)\cos\left(\frac{1}{2}\pi(y-L+2l)/(L-l)\right) & \text{in } G_2\\
-\cos\left(\frac{1}{2}\pi(x+L-2l)/(L-l)\right)\cos\left(\frac{1}{2}\pi(y-L+2l)/(L-l)\right) & \text{in } G_3\\
\cos\left(\frac{1}{2}\pi(x-L+2l)/L-l)\right)\sin(\pi|y|/l) & \text{in } G_4\\
0 & \text{in } G_5\\
\cos\left(\frac{1}{2}\pi(L-x-2l)/(L-l)\right)\sin(\pi|y|/l) & \text{in } G_6\\
2\sin\left(\frac{1}{4}\pi(x+y-2L+4l)/(L-l)\right)\sin\left(\frac{1}{4}\pi(x-y)/(L-l)\right) & \text{in } G_7\\
\sin(\pi|y|/l)\cos\left(\frac{1}{2}\pi(L-2l+x)/(L-1)\right) & \text{in } G_8\\
-\cos\left(\frac{1}{2}\pi(L-2l+x)/(L-l)\right)\cos\left(\frac{1}{2}\pi(L-2l+y)/(L-l)\right) & \text{in } G_9
\end{cases}$$

so that the initial crystal coincides with G_5. The character of this, accidentally chosen, temperature distribution compared the melting temperature $\vartheta = 0$ is shown in Fig. 6. Computations were performed in the following variants: 1. there is a prohibition of the phase transition $C_f \Rightarrow C_s$ outside of a boundary layer BF, separating the existing crystal from the bulk of the liquid phase and the threshold of undecooling is equal to $T_m = 0$; 2. the phase transition occurs in each region where conditions 1–4 of the introduction are valid; a: $\delta T_m = 0$ and b: $\delta T_m/T_m = 0.1$. Results of these computations are shown in Fig. 7, 8, 9. The sequence of the moments of phase transitions in the case 2, b is given in Table 3.

The process of the single crystal growth (case 1) is so rapid that the phase transitions are found at each time step. This means that the sequence of moments of phase transitions is in this case rather unreliable. Values of t^m are there estimated from above and the number of phase transitions — from below. The same relates to the initial stage of the process in case 2.

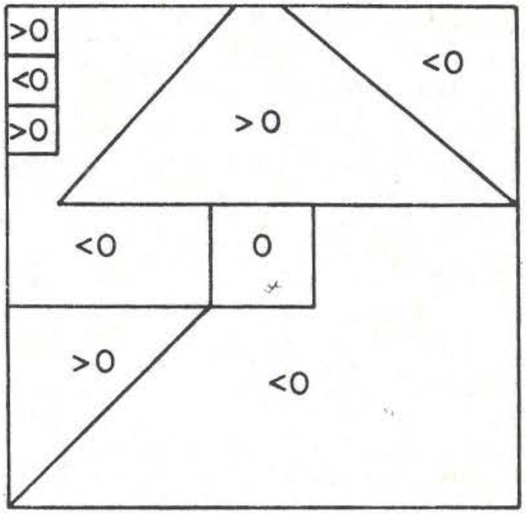

Fig. 6. Example 3. The initial field of temperature compared to the melting temperature

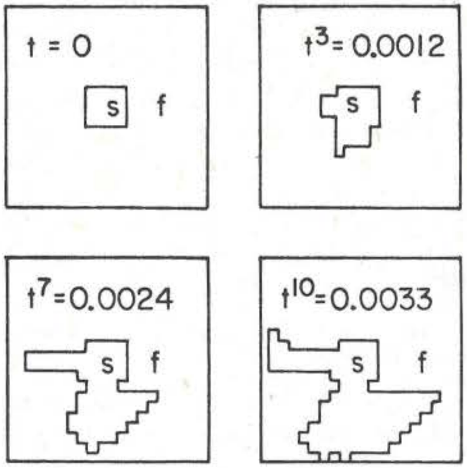

Fig. 7. The growth of a crystal immersed into a partly undercooled, partly overheated melt. Example 3. $T_m = 0$. No phase transition outside of BF

Table 3

The growth of crystals in a partly undercooled, partly overheated melt

Example 3

Case 2, b ($\tau = 0.0003$)

m	1	2	3	4	5	6	7	8	9
t^m	0.0003	0.0006	0.0009	0.0012	0.0015	0.0021	0.0024	0.0027	0.0030
m	10	11	12	13	14	15	16	17	18
t^m	0.0036	0.0039	0.0057	0.0063	0.0066	0.0069	0.0081	0.0096	0.0144
m	19	20	21	22	23	24	25	26	27
t^m	0.0171	0.0192	0.0216	0.0222	0.0249	0.0255	0.0282	0.0309	0.0474
m	28	29	30	31	32	33	34	The number of steps made after the last phase transition 13437	
t^m	0.0480	0.0597	0.1614	0.2010	0.2208	0.2889	0.4689		

5. The comparison with the classical Stefan approach. The influence of the latent heat of creation γ_{sf} of a plane phase-interface solid-liquid.

Example 4 is aimed to offer a comparison of our present approach and the enthalpy version of the classical Stefan one. Here $(x, y, 0)$ is taken equal to

$$\vartheta(x,y,0) = \begin{cases} -10\,(x^2-l^2)\,(y-h)\,l^{-2}\,h^{-1} & \text{for } -l < x < l;\, 0 < y < h \\ (x-l)(1+y/H)/(L-l) & \text{for } l < x < L;\, 0 < y < H \\ -(x+l)(2-y/H)/(L-l) & \text{for } -L < x < -l;\, 0 < y < H \\ (y-h)(l^2-x^2)\,l^{-2}\,(H-h)^{-1} & \text{for } -l < x < l;\, h < y < H \end{cases} \quad (28)$$

and the boundary temperature — coinciding with the limiting values of the initial temperature.

Note that the explicit finite difference scheme is not applicable for the solution of the two-dimensional Stefan problem due to the strong instability taking place even for time steps of several orders below those indicated by the usual criterion of stability. Therefore computations were performed by the use of Oleinik's method of smoothing the enthalpy function with the subsequent applying the Peaceman-Rachford algorithm (See Rubinstein, 1971).

Results of computations are shown in Fig 10 a, b. The Stefan approach shows a non-monotonic character of the process evolution. After the very short period of the crystal growth, begins its melting. In the contrast to this

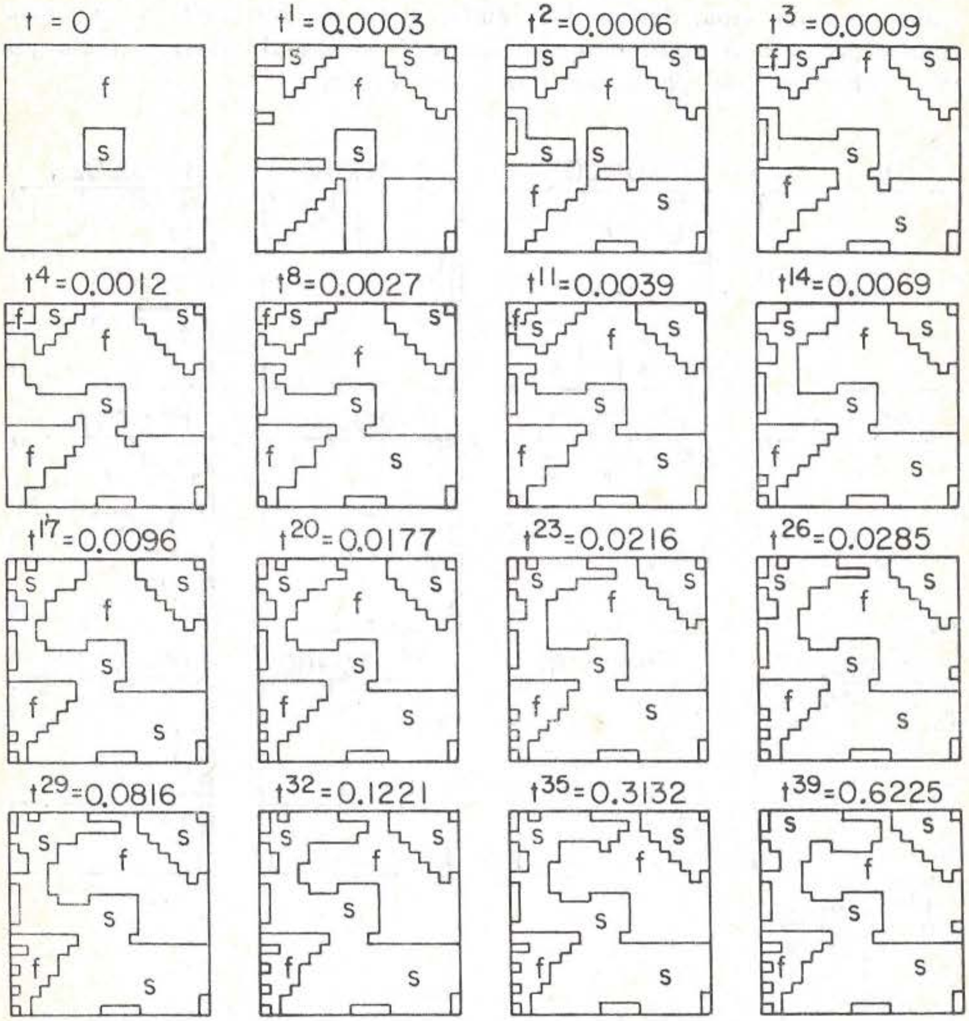

Fig. 8. The growth of a crystal immersed into a partly undercooled, partly overheated melt. Example 3. $\delta_{\downarrow} T_m/^{T}{}_m = 0$. Generation of new crystals is allowed

behaviour, in our approach the process of the crystal growth is monotonic. The computations do not show any tendency to the non-monotonicity.

Example 5 is destined to the consideration of the influence of the latent heat γ_{sf} of creation of plane phase-interfaces. As it has been mentioned in the introduction, this influence may be observable only for virtual crystallits several orders smaller than those we deal with, if the physically reasonable values of γ_{sf} are used for computations. In order to see the impact of γ_{sf} in our case we have performed computations with

$$\gamma_{sf} = 0.1 \cdot 10^{-3}; 0.376; .76 \text{ and } 37.6 \qquad (29)$$

using the same input data as in example 1. In the first case the complete coincidence with computations of example 1 is natural, whereas in the all three other cases no phase transitions were observed.

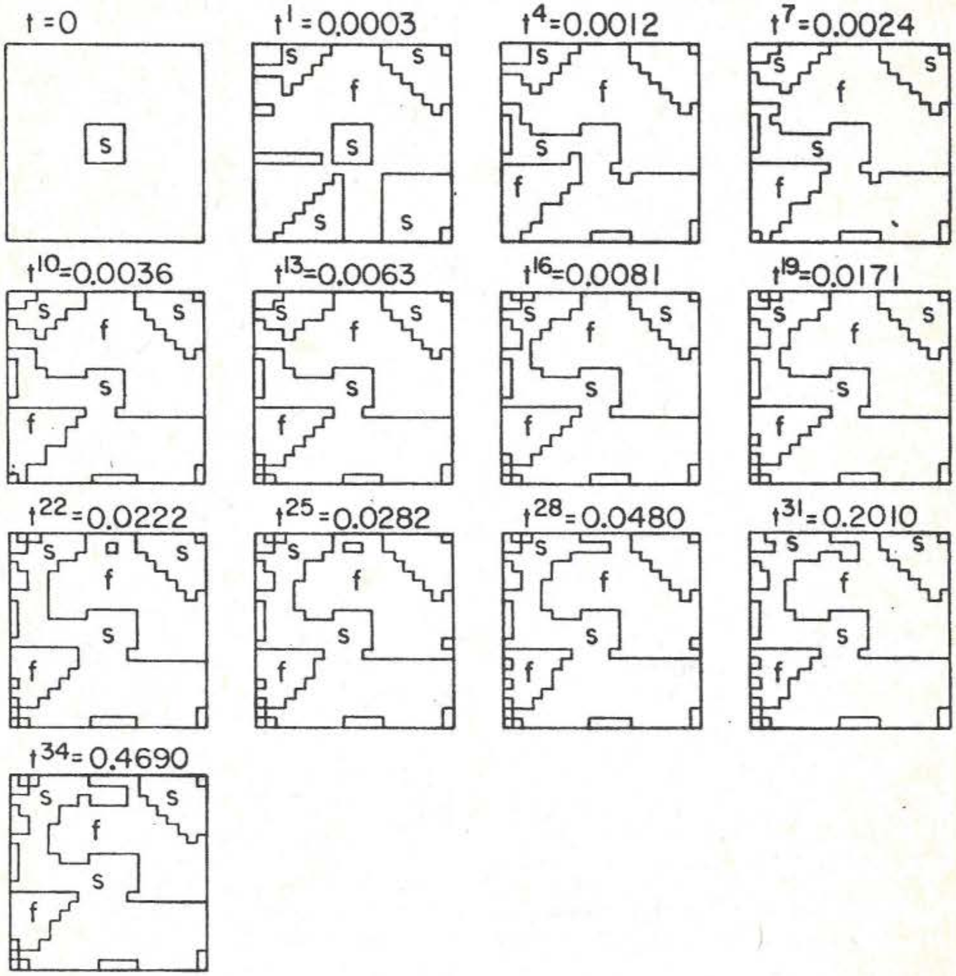

Fig. 9. The growth of a crystal immersed into a partly undercooled, partly overhead melt. Example 3. $\delta_{\downarrow} T_m/T_m = 0.1$. Generation of new crystals is allowed

6. Conclusion

As it has been emphasized above, our computations are only destined for illustration of the model proposed in (Rubinstein, 1983). However they may apparently help to derive some inferences concentrating the reasonableness of this model. Indeed, all the computations, described above, demonstrate the alteration of the process of the phase transition acceleration and its deceleration, and even stopping. Such a behaviour is a characteristic property of a real process of crystallisation (Chernov, 1962) and may therefore be considered as a strong evidence in favour of the model we deal with.

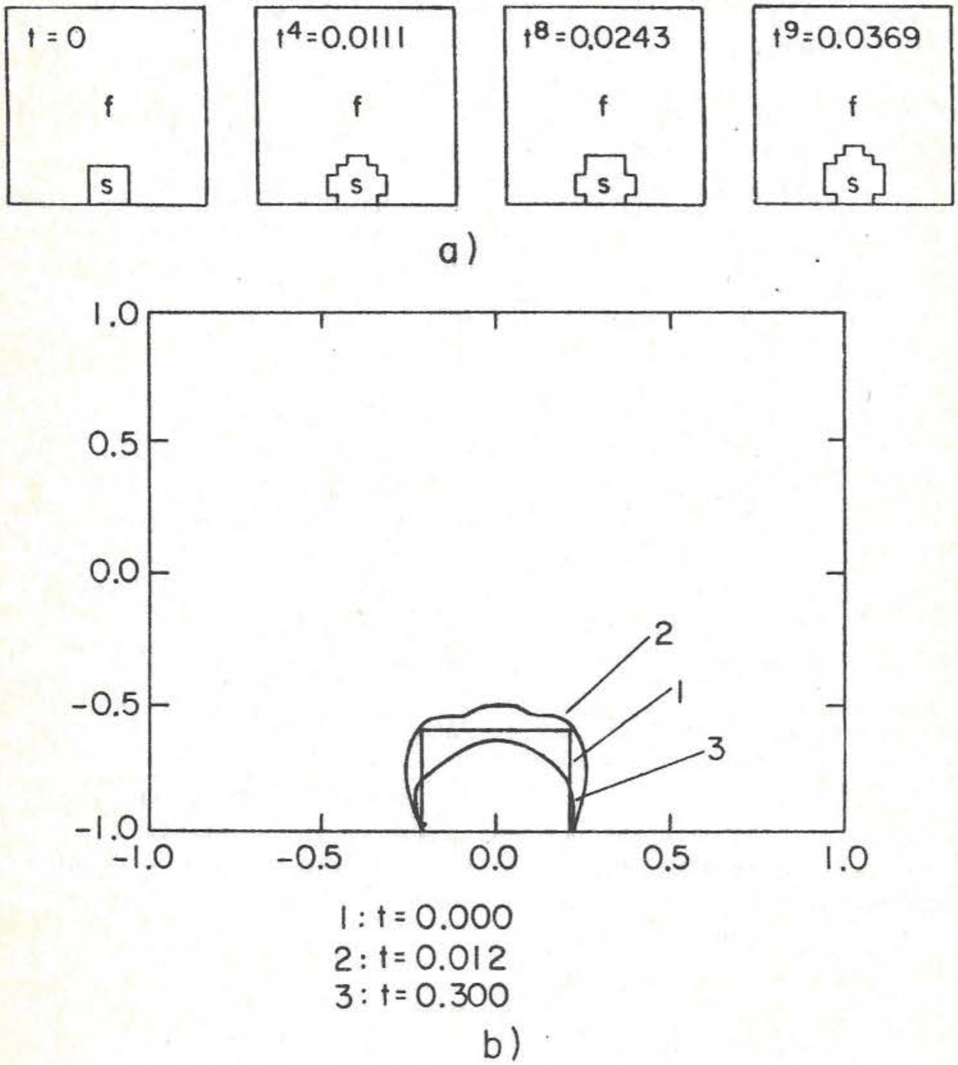

Fig. 10. The comparison with the Stefan approach. Example 4. a. Crystal growth according to the model of this paper. b. The Stefan approach

Results of computations performed with taking into account the impact of the latent heat of creation of plane interfaces solid-liquid strongly support the inference stated in the introduction concerning the importance of it in cases where the area of virtual crystallits is small enough compared with the length of their boundaries (i.e. when the latter is of order smaller than 1 micron). Moreover, it indicates the desirability of the corresponding alteration of the formulation of the classical Stefan problem. Indeed, in its well know formulation (Langer, 1980), the distinction of the melting temperature on the surface of a non-zero mean curvature and that on the plane phase-interfaces is only taken into account. The latent heat of creation of new plane phase-interface has been never considered in Stefan problem and its generalization.

Finally, we have to emphasize that our computations have demonstrated a serious qualitative difference between our and the classical Stefan approach. In example 4 the enthalpy version of the classical Stefan approach has demonstrated not monotonic development of the process whereas in our model the computation has shown the very rapid stopping of the evolution of the process of the change of the phase state without any evidence of the nonmonotonicity of this process.

Nevertheless we have to emphasize that all our conclusions are the results of computations performed for the system with really macroscopic size of virtual crystallits. For more realistic judgment one has to deal with crystallits of a minimal physically admissible size. The latter may be estimated as a value of order of several tens Angstrom since the macroscopic equation of heat conduction is applicable to bodies of such size and the applicability of this equation to bodies of essentially smaller size is questionable. The reduction of the virtual crystallit sizes up to such values would require a radical change of the applicable algorithm. One may think that in such a case Monte-Carlo method would be preferable.

We have to emphasize that we have no wish to overestimate the significance of the model we deal with. The real process of crystallization evolves on a microscopic level with its simultaneous subordination to the macroscopic conditions of the heat and mass transfer in bulks of both phases. The more adequate theory has to take into consideration both the microscopic and macroscopic subprocesses. The creation of such a theory is the matter of future.

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Ilustracje numeryczne artykułu "O modelowaniu matematycznym wzrostu pojedyńczego jednoskładnikowego kryształu z wytopu w niejednostajnym polu temperaturowym"

Praca zawiera ilustracje numeryczne do artykułu [Rubinstein, 83], dotyczące zaproponowanego tam makroskopowego modelu wzrostu kryształu.

Численные иллюстрации к работе „О математическом моделировании роста отдельного монокомпонентного кристалла с расплава в неоднородном температурном поле"

Работа содержит численные иллюстрации касающиеся макроскопической модели роста индивидуального кристалла из мельта, предложенные в публикации [Рубинштейн, 83].

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