Quantitative isothermal phase-field simulations of peritectic phase transformation in Fe–Mn system

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A B S T R A C T
The present investigation shows quantitative results for the peritectic phase transformation of Fe–Mn alloys utilizing phase-field simulations in 1-D and 2-D. The phase-field method used was based on an adaptation of the proposal of Folch and Plapp [Phys. Rev. E, 2005, 72, 011602] for the eutectic reaction. The two stages of peritectic phase transformation, the peritectic reaction and the peritectic transformation, were investigated numerically utilizing this phase-field approach. The evolution of the phases was quantitatively analyzed during the peritectic transformation and the fractions of the phases at the end of the solidification were compared with the thermodynamic equilibrium, defined by the phase diagram, for the case of 1-D simulation with peritectic concentration. An assessment of the behavior of the concentration gradient in the γ-phase (the peritectic phase) through time was also carried out and a mathematical function which describes the γ-phase thickness evolution was defined. Finally, 2-D simulations were performed to clearly identify the two stages of the peritectic phase transformation. The obtained results show two main facts: (1) the numerical model is able to simulate quantitatively this phase transformation; and, (2) this numerical tool can be utilized for investigating quantitatively some aspects (normally determined indirectly) that are difficult to be determined by direct measurements in experimental works.

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1. Introduction

Solidification processes have been extensively researched over more than four decades in order to deeply understand the behavior of microstructure evolution and how the process parameters influence the solidified structure. Much progress in this direction has been observed in the literature and a fact, which can be highlighted, is the development of rigorous analytical models for microstructure evolution under steady-state and non-steady-state conditions [1–6]. In this context, a metallurgical topic, which has received considerable attention for many years and will be explored here is the peritectic phase transformation. According to the nomenclature proposed by St. John [7], this phase transformation can be divided into two parts, peritectic reaction and peritectic transformation. The
term “peritectic reaction” will be used to define the reaction stage in which the “collar” of the new phase (the peritectic phase) is in formation. In this stage, there is still the existence of a real contact between the three phases (triple point). The term “peritectic transformation” will be utilized for the reaction stage that happens after the peritectic reaction, when there is no triple point anymore. In this latter stage, the advance of the reaction is controlled essentially by solid state diffusion through the “collar” of \( \gamma \)-phase. The solute present in the liquid phase is gradually transferred into \( \delta \)-phase direction, whereas the “collar” of \( \gamma \)-phase thickens by its growth simultaneously into the liquid phase and into the \( \delta \)-phase. Fig. 1 displays a sketch of the two stages of the peritectic phase transformation and some results of direct observation of the peritectic phase transformation from Ref. [8].

Some researches in solidification field have utilized numerical tools for simulating solidification phenomena and quantifying important metallurgical properties [9–12] such as primary and secondary dendrite arm spacing \( (\lambda_1, \lambda_2) \), phase distribution, as well as macro- and micro-segregation patterns. In this context, one of the most prominent methods for simulations of solidification is widely known as “phase-field method” (PFM). This method has been utilized for qualitative and quantitative evaluation in both cases: single solid phase forming from liquid [13–18] and peritectic or eutectic phase transformation [19–24].

Therefore, the PFM was applied in the present investigation to simulate the peritectic phase transformation under isothermal solidification conditions with small undercooling. It was possible, with this method, to quantify kinetic aspects of the peritectic transformation and to observe clearly the occurrence of the two stages of the peritectic phase transformation. Simulations in 1-D and 2-D were performed with the numerical model. The investigated alloys were binary alloys in the region of the peritectic phase transformation of the Fe–Mn system. These alloys were selected since the peritectic phase transformation is also observed in medium manganese steel (MMnS) grades and in high manganese steel (HMnS) grades being developed in the last 15 years. The choice for the present PFM approach was based on the fact that there is in the literature a quantitative numerical model for eutectic phase transformation [19]. This model was developed in a general way, being applicable to any phase transformation involving simultaneously two solid phases and the liquid phase. Thus, the present work adapted this approach from eutectic phase transformation to peritectic case.

The phase’s evolution during the phase transformation was investigated for the case of 1-D simulations and kinetic aspects of the phase transformation were also determined for these simulations. The results of 1-D simulations were compared, at the end of phase transformation, with the phase fractions defined by thermodynamic equilibrium (based on the phase-diagram). In addition to that, the behavior of the concentration gradient in the \( \gamma \)-phase during the peritectic transformation was also assessed and a mathematical function of the \( \gamma \)-phase thickness evolution was determined. Finally, the 2-D numerical simulation was performed to evaluate the occurrence firstly of the peritectic reaction and afterwards of the peritectic transformation as proposed by literature [7].

2. Peritectic phase-field model for isothermal solidification

By following the proposed models of [14,15], the description of the thermodynamic equilibrium in the bulk and interface regions can be defined based on linearization of the phase diagram lines. Thus, in the present approach, the phase diagram was described by straight liquidus and solidus line of slopes \( m \) and \( m/k \), respectively. This fact helps significantly on the description of phase-field equations and the numerical treatment. The detailed analysis of sharp-interface and phase-field models for solidification can be found in Refs. [14–16] for dilute
binary alloys and for pure substances [17, 18]. These models are for the cases of a single solid phase growing from the liquid phase. Based on the methodology proposed in Refs. [14–18], Folch and Plapp [19] were able to extend a binary phase field model to the case of two solid phases together with the liquid phase. Thus, they simulated quantitatively the eutectic phase transformation. They have also demonstrated that the numerical results from the simulations agreed with the results of a traditional analytical model. Therefore, since Folch and Plapp's model was effective in the quantitative simulation of solidification for more than one solid phase, the same model was selected here for exploring the peritectic phase transformation.

After applying the variational formulation that is well-described in Ref. [19] and assuming that the three phases have the same interfacial energy \( \gamma_3 = \gamma_\gamma = \gamma_L = \gamma \), the mathematical equation which describes the evolution of the phase-field variables, \( p_i \), with \( i = \delta, \gamma, L \), can be defined by

\[
\frac{\delta (p_i)}{\delta t} = \nabla^2 p_i + \frac{2}{3} (\bar{p} - p_i (1 - p_i) (1 - 2p_i) + p_i (1 - p_i) (1 - 2p_i)) + \sum_j \frac{\delta p_j}{\delta p_i} \left\{ (\mu A_j - B_i) \right\}
\]

(1)

This numerical model follows the restriction on the phase-field variables proposed by Steinbach and co-authors [25], that is \( p_\delta + p_\gamma + p_L = 1 \). In addition to that, for the present approach \( p_i \in [0, 1] \forall i \) and the three phase-field variables can be denoted by \( \bar{p} = (p_\delta, p_\gamma, p_L) \). Eq. (1) includes already all the conversions proposed in Refs. [14–19] for making the differential equations dimensionless.

The function \( g_i \), which appears in Eq. (1), is determined by:

\[
g_i = \frac{p_i^2}{4} [15 (1 - p_i) (1 + p_i - (p_k - p_j)^2 + p_i (9p_i^2 - 5))]
\]

(2)

The complete description of variables of the equations can be found in Table 1, when the description is not in the text. The variable \( \lambda \) is defined by

\[
\lambda = \frac{W a_1 d}{d_\delta + d_\gamma} = \left( \frac{1}{|A_i - A_L|} + \frac{1}{|A_\gamma - A_L|} \right),
\]

where \( a_1 \) is a constant with value equal to 0.4584, according to Ref. [19], and \( d = 0.5 \cdot (d_\delta + d_\gamma) \).

Table 1 – Description of model variables.

| \( \xi \) | Normalized concentration |
| \( C \) | Concentration, wt.\% |
| \( T \) | Temperature, K |
| \( T_p \) | Peritectic temperature, K |
| \( \xi \) | Dimensionless simulation time |
| \( \mu \) | Dimensionless chemical potential |
| \( W \) | Interface thickness, m |
| \( d_i \) | Capillary length of \( \delta \) and \( \gamma \) phase, m |
| \( k_i \) | Partition coefficient |
| \( m_i \) | Slope of liquidus line for \( \delta \) and \( \gamma \) phase, K/wt.\% |

Fig. 2 – A sketch of a two component phase diagram for the peritectic reaction.

The terms \( A_i \) and \( B_i \) are functions of temperature and determine the thermodynamic equilibrium observed in the phase diagram, which follows the sketch of Fig. 2 for the region of peritectic phase transformation. The definition of these functions for isothermal analyses of \( \delta \) or \( \gamma \)-phase is expressed by

\[
A_i = c_i + \frac{(1 - k_i) (T - T_p)}{m_i |\Delta C|}
\]

(4)

\[
B_i = A_i \frac{T - T_p}{m_i |\Delta C|}
\]

(5)

The normalized concentration, \( c_i \), used in Eq. (4) is determined by

\[
c_i = \frac{C_i - C_P}{\Delta C}
\]

(6)

\( \Delta C = C_L - C_\delta \); the \( A_L \) and \( B_L \) are equal to zero. The dimensionless chemical potential, \( \mu \), and the concentration are related one to another by

\[
\mu = \xi - A_i p_\delta - A_\gamma p_\gamma - A_L p_L
\]

(7)

Based on the nonvariational formulation proposed in Ref. [19], the evolution of \( \mu \) can be defined by

\[
\frac{\delta \mu}{\delta t} = \nabla \cdot \left( \frac{D_\delta p_\delta + D_\gamma p_\gamma + D_L p_L}{|\nabla p_i|} \nabla \mu \right) - \sum_i A_{i} \frac{\delta p_i}{\delta t}
\]

(8)

\[
+ 2 \cdot \alpha \cdot \sum_{i=1}^{3} (A_i - A_L) \left( - \frac{\nabla p_i}{|\nabla p_L|} \cdot \nabla \mu \right) \cdot \left( \frac{\nabla p_i}{|\nabla p_L|} \cdot \frac{\delta p_i}{\delta t} \right).
\]

already including in its formulation the anti-trapping current.

The variables \( D_\delta, D_\gamma \) and \( D_L \) mentioned in Eq. (8) are the dimensionless diffusion coefficients, respectively, in the liquid phase, in the \( \delta \)-phase and in the \( \gamma \)-phase. Further details of the present formulation can be found in Ref. [19].
3. Materials and measurement methodology

To obtain suitable values for the simplified liquidus slopes of δ-phase and γ-phase (m₁ and m₂), and for the partition coefficients (k₁ and k₂) in Fe–Mn system, the phase diagram was obtained from Thermo-Calc® [26] (thermodynamic database TCREF). Linear regressions were performed for the liquidus lines of δ-phase and γ-phase and on this basis, the liquidus slopes were defined for both phases. The values of the liquidus slope for δ-phase and for γ-phase were equal to −5.29 K/wt.% and −4.05 K/wt.%, respectively. The definition of the partition coefficients for both phases was made through averaging many measurements for the ratio of the solid concentration (in equilibrium with the liquid) to the respective liquid concentration from the Thermo-Calc® lines. For the case of δ-phase, the region considered was [Tₚ, Tₚ + 10]. For the case of γ-phase, the region considered was [Tₚ − 10, Tₚ]. The obtained values were: k₁ = 0.724 and k₂ = 0.821.

Table 2 presents the numerical data used in the simulations (please refer to Fig. 2 for further details). The diffusion coefficients correspond to the value at the peritectic temperature. The diffusion data for γ-phase was taken from DICTRA® [27] (thermodynamic database TCREF, mobility database MOB2), for δ-phase from Ref. [28] and for the liquid phase from Ref. [29].

The capillary length for δ-phase and for γ-phase follows the definition of Ref. [19]. The dimensionless grid spacing, Δx̅, utilized for the simulations was set equal to 0.80 and the dimensionless time increment, Δt̅, has followed the proposal of Refs. [14,15].

The simulation utilizing the 1-D numerical model was carried out for the peritectic concentration (10.1 wt.% of Mn) and the numerical domain dimension was equal to 162 µm (160-W). In the beginning of the simulation, the solid fraction of δ-phase was preset in accordance to the phase diagram exactly at the peritectic temperature and a small nucleus of γ-phase was positioned on the δ-liquid interface. Fig. 3 shows a sketch of this initial condition. This pattern was selected to simulate the isothermal peritectic transformation under low undercooling. With this proposed pattern, in 1-D, there was no initial contact between the three phases. The simulation was performed until the total amount of solid phase being higher than 99.7%. This 1-D pattern can be interpreted as the radial growth of a circle for 2-D or a sphere for 3-D, by assuming the diffusion only in the same direction.

Table 2 – Alloy and numerical parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concentration of δ-phase, Cₓ</td>
<td>8.9 wt.% of Mn</td>
</tr>
<tr>
<td>Peritectic concentration, Cₚ</td>
<td>10.1 wt.% of Mn</td>
</tr>
<tr>
<td>Concentration of liquid-phase, Cₑ</td>
<td>12.3 wt.% of Mn</td>
</tr>
<tr>
<td>Peritectic Temperature, Tₚ</td>
<td>1473 °C</td>
</tr>
<tr>
<td>Capillarity length of δ-phase, dₓ</td>
<td>2.01 × 10⁻⁶ m</td>
</tr>
<tr>
<td>Capillarity length of γ-phase, dₑ</td>
<td>3.11 × 10⁻⁶ m</td>
</tr>
<tr>
<td>W/dₓ</td>
<td>39.56</td>
</tr>
<tr>
<td>Undercooling, Tₚ − T</td>
<td>1.0 K</td>
</tr>
<tr>
<td>Mn diffusion coefficient in the liquid phase, Dₓ</td>
<td>2.7 × 10⁻⁹ m²/s</td>
</tr>
<tr>
<td>Mn diffusion coefficient in δ-phase, Dₓ²</td>
<td>2.5 × 10⁻¹² m²/s</td>
</tr>
<tr>
<td>Mn diffusion coefficient in γ-phase, Dₑ²</td>
<td>3.0 × 10⁻¹² m²/s</td>
</tr>
</tbody>
</table>

![Fig. 3 – Initial condition of 1-D simulation.](image)

By using the proposed 1-D simulation, the phase present in each cell of the simulation domain was determined by the highest value of pₓ inside the cell, e.g., if pₓ was the highest value of a specific domain cell then the latter was considered a δ-phase cell. This procedure was carried out for the different simulation times on the whole domain and an estimative of the thickness of each phase was determined by counting separately the number of cells of δ-phase, γ-phase and liquid. Thus, it was possible to assess the kinetic of phases evolution.

An analysis of the concentration profile inside the whole numerical domain was made for different simulation times. This assessment was developed plotting the concentration of manganese versus the domain dimensionless length (η = z/w). After observing changes in the concentration gradient inside γ-phase, the slopes of the concentration gradient inside this phase were determined using linear regressions and the behavior of this with time was also assessed.

Refs. [30–32] suggest that the evolution of the γ-phase thickness, ε(t), follows the mathematical equation defined by

\[ ε(t) = A t^n \]  

(9)

Thus, the coefficients A and n of Eq. (9) from the numerical simulation were determined by linear regression of the natural logarithm of γ-phase thickness versus natural logarithm of time for the numerical data obtained by the simulation. Additionally to 1-D simulation, two 2-D simulations of hyperperitectic alloys were performed with the same model in order to investigate the occurrence of peritectic reaction followed by peritectic transformation. The first simulation was performed without anisotropy and it was carried out by introducing a circular region of δ-phase inside the liquid phase with a small nucleus of γ-phase on the δ-liquid interface (Fig. 7(a)). This alloy has concentration of 12.2 wt.% of manganese and the numerical domain was square with lateral length equal to 162 µm (160-W). The second simulation was performed considering the anisotropy effect and the alloy concentration was equal to 11.6 wt.% of manganese. The nucleation of the γ-phase took place on the δ-liquid interface, similar that of the first simulation. The numerical domain was also square with lateral length equal to 243 µm (240-W).

4. Results and discussions

4.1. One dimensional simulation

Fig. 4 shows the time evolution of the δ-phase, of the γ-phase and of the total amount of solid phase for the Fe–Mn peritectic alloy obtained by the results of 1-D numerical simulation. The amounts of the phases shown on the diagram correspond to
volume fractions. The evolution of the total amount of solid phase is shown by the small squares and it was defined by the sum of δ-phase and γ-phase fractions. The liquid phase was omitted because its fraction can be determined by the difference between one hundred (percent) and the solid phase fraction.

The results of Fig. 4 show that the fraction of γ-phase is very close to zero in the beginning of the phase transformation, which corresponds to the nucleation period. After that, the γ-phase grows into the liquid phase and also into the δ-phase, according to the description of peritectic phase transformation. The result of the numerical simulation, depicted in this figure, shows exactly this behavior because a reduction of δ-phase amount together with an increase of the solid phase amount can be observed through the time evolution. Furthermore, it is also possible to observe in Fig. 4 that the evolution of the phases through the time follows an asymptotic function, which is typically observed in a phase transformation controlled by diffusion. In the beginning of the phase transformation, the growth rate of γ-phase is potentially higher than the growth rate in the intermediate or in the final stages of the phase transformation. A similar asymptotic behavior can also be observed for the δ-phase but leading in the case of the δ-phase to a progressive reduction of its phase fraction.

The reason for the asymptotic behavior of the phases through time observed in Fig. 4 can be explained by the first Fick's law, which defines the flux of a “B” solute by \( J_B = -D_B(\Delta C_B/\Delta x) \) in 1-D. By supposing that both the concentration of δ-phase next to the δ-γ interface and the concentration of liquid phase next to liquid-γ interface are unchangeable during steady-state growth, it follows that, the concentration difference inside the γ-phase between the two interfaces (with δ and liquid phases) can be considered constant in steady-state. Taking into account the later assumption (\( \Delta C_{Mn} \approx \) Constant) and by considering that the diffusion coefficient is constant for the isothermal simulation, it may be concluded that the solute flux decreases over time, since there is a growth of γ-phase layer (an increase of Δx). Since this solute-flux is the rate-controlling process of the peritectic transformation, the γ-growth rate must also steadily decrease.

In order to gain insight into the asymptotic shape of the curves observed in Fig. 4, an analysis of the concentration profile inside the phases for different time-steps was developed and the first results are depicted in Fig. 5. From the left to the right, the δ-phase is characterized in this figure by the region possessing the lowest concentrations, around 8.9 wt.% of manganese. The γ-phase region is defined by the region with manganese contents about 10.1 wt.% and showing an important positive concentration gradient inside it and finally, the liquid is positioned in the region of the numerical domain corresponding to a concentration of ca. 12.6 wt.% of manganese. The regions with appreciable concentration jumps (increases or decreases) correspond to the interface regions.

Four main points may be mentioned based on the results presented in Fig. 5. The first interesting one is that the concentration inside the δ-phase far away of δ-γ interface shows a small reduction with time evolution. This happens because there is a reduction of the manganese content next to the δ-γ interface, which in its turn causes a concentration gradient inside the δ-phase region. This concentration gradient inside the δ-phase creates an energetic difference, which tends to homogenize the δ-phase, its concentration converging to a spatially constant value, the composition of the δ-phase in equilibrium with the γ-phase. Further homogenization is accomplished through manganese diffusion into the δ-γ interface. Therefore, with the progress of simulation time, a depletion of manganese in δ-phase is observed and the concentration achieved in δ-phase is exactly the concentration of δ-phase next to the δ-γ interface in steady-state. The second fact to be noticed in the results of Fig. 5 is that the concentration profile inside the γ-phase follows a linear behavior with low concentration next to the δ-γ interface and with

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Fig. 4 – The phase fractions versus time for a Fe–Mn peritectic alloy with 10.1 wt.% of Mn.

Fig. 5 – Concentration profiles of Mn inside of the simulated numerical domain at different time-steps.
Fig. 6 – The concentration gradient inside the γ-phase through the time. The term \( \gamma \) means dimensionless length \((2 \cdot W^{-1})\).

The behavior through time of the concentration gradient inside the γ-phase \((dC/d\eta)\) was assessed and the corresponding results are depicted in Fig. 6. "\( \eta \)" expresses the dimensionless length. The results of this figure show quantitatively that the concentration gradient inside the γ-phase also follows the shape of an asymptotic function. This fact evidences that the peritectic phase transformation is being controlled by diffusion and that the mathematical model presented here is able to reproduce reasonable quantitative results in what concerns this phase transformation.

The concentration gradient inside γ-phase tends to zero when the degree of homogeneity of γ-phase increases, according to the results of Fig. 6. The complete homogeneity will be achieved only if there is no δ-phase in the simulation domain and with a long simulation time in order to guarantee the complete homogeneity of the simulated peritectic alloy. The complete homogenization of γ-phase is not observed in our simulation because the simulation was stopped when the solid fraction achieved a value higher than 99.7%. In the absence of the liquid phase, the δ–γ interface migration becomes sluggish. Probably, if the simulation had been continued after the complete solidification, it would have been possible to observe a complete γ-transformation and a higher homogenization degree of the γ-phase.

After obtaining the simulation results and plotting the natural logarithm of γ-phase thickness versus natural logarithm of time, the parameters \( A \) and \( n \) of Eq. (9) were determined and the function expressing the γ-phase thickness evolution, which resulted was

\[
\epsilon(t) = 3.4674 \cdot t^{0.3911}
\]

(10)

where \( \epsilon(t) \) is expressed in \( \mu m \) and the time in minutes. Although Eq. (10) does not correspond to a square root function as proposed by some analytical models in the literature [7,30,32], the parameters \( A \) and \( n \) are situated in the range of the experimental values also reported in the literature for other alloys [31]. Besides that, in [30] the authors consider that values of \( n \) from 0.35 to 0.57, though not corresponding to the parabolic law, would still be compatible with the kinetics of peritectic growth.

From the expressions in Ref. [32], it is clear that the thickness evolution over time for the case of one-dimensional planar growth during the peritectic transformation is only expected to follow a parabolic law when the diffusion in the liquid and in the properitectic phase may be neglected: e.g., in the case where there is a perfect homogenization of the liquid through convection and the composition of the properitectic phase is fixed. In all other cases (including the present one) deviations from a parabolic law may be expected.

According to the equilibrium phase diagram, the only phase that should be present at the end of solidification is the γ-phase for the peritectic alloy. Nevertheless, the phase fraction observed in Fig. 4 at the end of solidification is 92.1% of γ-phase and 7.6% of (residual) δ-phase. It shows that the complete equilibrium was not achieved for the system, even though a long dimensional time has been utilized in the simulation (dimensional time comparable with, or longer than, the solidification time of large and extra-large ingots). At the same time, the results show that the numerical model follows with a reasonable precision the thermodynamic equilibrium defined by phase diagram.

![Fig. 7 – The time evolution of the peritectic phase transformation in 2-D without anisotropy.](image)
4.2. Two dimensional simulations

The 2-D microstructures from the simulations at different time-steps are depicted in Figs. 7 and 8 for hyperperitectic alloys with 12.2 wt.% and 11.6 wt.% of manganese, respectively. The results of Fig. 7 were obtained for the case without the anisotropic growth effect and the results of Fig. 8 for the case with anisotropy. The δ-phase region is represented by the dark gray, the liquid region by the light gray and the γ-phase region by the black color. It is possible to observe in the results of Figs. 7 and 8 the two stages of the peritectic phase transformation, at first the peritectic reaction (Figs. 7b, 8b and c) and after that the peritectic transformation (Figs. 7c, 7d and 8d). For the peritectic reaction, the growth of γ-phase on the δ-phase can be clearly observed. This fact is in accordance with the theoretical description and also with the experimental observations at a temperature close to the three-phase equilibrium (Fig. 1b). For the peritectic transformation, it is possible to see the thickening of the γ-phase through time based on the growth of the same phase simultaneously into the liquid region and into the δ-phase region (compare Fig. 7c and d). Another fact that may be observed in the results of Figs. 7 and 8 is that the peritectic reaction happens much faster than the peritectic transformation. This fact can be explained by the following reasons: (1) the liquid diffusion coefficient is much higher than the solid diffusion coefficient for substitutional alloys, thus, the liquid situated in the region of the triple point has always concentrations favorable to the growth process of γ-phase due to the high solute mobility in the liquid phase; (2) according to Hillert [34], the diffusion distance inside the γ-phase is the shortest at the γ-tip advancing along the δ-liquid interface, therefore, the solid diffusion necessary for the progress of the phase transformation is considerably faster at the triple point region due to the very thin layer of γ-phase; (3) the peritectic transformation is completely controlled by the solid diffusion through the thickness of the γ-phase what makes the phase transformation rate much lower, analogously to the 1-D case.

5. Summary and conclusions

The phase-field approach presented here to simulate the peritectic phase transformation is consistent with the description of this phase transformation proposed in the classical papers about the subject, both concerning its thermodynamics and kinetics. The following arguments can be pinpointed in this respect:

- The numerical results of phase fractions at the end of the solidification follow with a reasonable precision the thermodynamic equilibrium defined by the phase diagram. Some small deviations observed in the results can be explained by kinetic effects;
- The simulation results for the evolution of phase fractions during the peritectic transformation show an asymptotic behavior compatible to the one observed in phase transformation controlled by diffusion. In addition to that, the shape evolution of the concentration gradient inside the γ-phase over time has also a characteristic asymptotic behavior, which evidences the ability of the model to simulate quantitatively the second stage of peritectic phase transformation based on the diffusion of solute through the γ-phase, from the liquid to the δ-phase;
- In the case of 2-D results, the occurrence of the two stages of the peritectic phase transformation during the solidification process, the peritectic reaction and the peritectic transformation, was clearly observed. The latter point shows that the model by itself has the ability of describing the favorable reaction sequence, in the first stage, the peritectic reaction and afterwards, in a second stage, the peritectic transformation.

A novel aspect put forward by this investigation is the quantitative assessment, through simulation, of a kinetic law for the peritectic transformation. The mathematical relation, which describes the γ-phase thickness evolution with time for the 1D case, though not a parabolic one, has mathematical coefficients comparable with experimental works. This indicates that phase-field simulations in 2D and 3D may possibly clarify various aspects of the kinetics of the peritectic reaction.

The presented facts help to clarify that the phase-field approach may be utilized to investigate some aspects which are difficult or, in some cases, impossible to be determined through experiments by direct measurements. Two examples of this point are the determination of the asymptotic behavior of the concentration gradient inside the γ-phase, measured in the simulations quantitatively and directly on the phase, and the occurrence of a concentration gradient inside the δ-phase in the first stages of the peritectic transformation. It

Fig. 8 - The time evolution of the peritectic phase transformation in 2-D with anisotropy.
is well-known that, normally, the asymptotic behavior of the concentration gradient inside the $\gamma$-phase is inferred indirectly in experimental works from the asymptotic behavior of the $\gamma$-phase thickness evolution with time. Nevertheless, in the present investigation the concentration gradient inside the $\gamma$-phase was quantitatively assessed independently of the $\gamma$-phase thickness evolution.

**Conflicts of interest**

The authors declare no conflicts of interest.

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**References**