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MODELLING OF MULTICOMPONENT DIFFUSIVE PHASE TRANSFORMATION IN SOLIDS*

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Abstract

Physical analysis of phase transformation of materials consisting from several (both substitutional and interstitial) components, coming from the Onsager extremal thermodynamic principle, leads, from the mathematical point of view, to a system of partial differential equations of evolution type, including certain integral term, with substantial differences in particular phases (α, γ) and in moving interface of finite thickness (β), in whose center the ideal liquid material behaviour can be detected. The numerical simulation of this process in MATLAB is able to explain some phenomena (e.g. the interface velocity as a function of temperature) better than known simplified models assuming the sharp interface and additional boundary and transfer conditions.

1. Introduction

The simulation of diffusional phase transformation requires to solve the coupled problem of bulk diffusion and interface migration. Most models pay attention especially to binary (two-component) alloys with substitutional components – cf. [1] and [6]. Usually the interface is assumed to be sharp (in other word: its thickness is supposed to be negligible), thus some artificial boundary and transfer conditions have to be applied at the interface, as e.g. the ortho- or para-equilibrium contact conditions for a multi-component model in [10]. However, a real migrating interface of finite thickness h may drag segregated impurity atoms forming concentration profiles across the interface. Such a local diffusion process reduces the migration velocity v due to the Gibbs energy dissipated by this process; this decelerating effect is known as solute drag. In this paper we shall consider alloys with a finite number (at least two) of components. In [11], following some ideas of [8], coming from the Onsager extremal thermodynamic principle (derived originally in [7], for more details and various generalizations see [5]), the steady-state diffusion of solute across the interface is driven by the difference of chemical potentials $\mu(c^\star)$, corresponding to the vector $c^\star$ of mole fractions (as concentrations characteristics) related to all q substitutional components, e.g. $c^\star = (c_1, \ldots, c_q)$; since $c_1 + \ldots + c_q = 1$, it is useful to introduce $c = (c_1, \ldots, c_{q-1})$, too. As discussed in [2], at least for the steady-state case this approach gives identical results with the solute drag formula proposed in [4]. In [15] the same approach is generalized to admit the evolution of molar fractions in time

and the presence of r interstitial components; consequently $c^\star = (c_1, \ldots, c_q, \ldots, c_{q+r})$ and $c = (c_1, \ldots, c_{q-1}, c_{q+1}, \ldots, c_{q+r})$. Nevertheless, [15] shows only one practical example of such evolution near the initial time; the algorithm suggested in this paper handles also slow long-time redistributions.

All material characteristics (chemical potentials, diffusion factors, interface mobility) should correspond to a material structure where usual lengths are in micrometers; moreover, the usual interface thickness can be 10^{-10} m. Consequently, it is not easy to identify such characteristics in the laboratory. This is the first reason for the one-dimensional formulation of the problem in this paper, the second one is the requirement of simple, transparent and reader-friendly notations; some useful generalizations will be sketched in concluding remarks. For certain material sample of length H, in addition to $c^\star$ and c it is useful to introduce vectors of diffusive fluxes $j^\star = (j_1, \ldots, j_q, \ldots, j_{q+r})$ where $j_1 + \ldots + j_q = 0$. We shall study the redistribution of c and j in an arbitrary positive time t in a closed system with $j(.) = 0$ at the boundary (consisting of two points, whose distance is H). Such system requires no additional boundary conditions; we need only to know all initial values c for $t = 0$. If x refers to the standard Cartesian coordinate system and v is positive for the interface motion from the left to the right we can localize the interface (for x) into the interval $\langle 0, h \rangle$ and the exterior boundary of a sample into two points

$$x_L(t) = x_L(0) - \int_0^t v(\varsigma)\,\mathrm{d}\varsigma \qquad x_R(t) = x_R(0) - \int_0^t v(\varsigma)\,\mathrm{d}\varsigma\,;$$

clearly $x_R(t) - x_L(t) = H$ and $j(x_L) = j(x_R) = 0$ for any t. Finally we have the first phase, denoted in all following considerations by α, for $x < 0$, separated from the second phase, denoted by γ, for $x > h$, by the phase interface, denoted formally by β, for $0 \leq x \leq h$.

If the dot symbol denotes the partial derivative with respect to t and the prime symbol the partial derivative with respect to x then we are able to calculate the total time derivative of a variable u as $\mathrm{d}u/\mathrm{d}t = \dot{u} - vu'$. Namely the mass conservation law for the constant molar volume Ω reads

$$\mathrm{d}c^\star/\mathrm{d}t + \Omega j^{\star\prime} = \dot{c}^\star - vc^{\star\prime} + \Omega j^{\star\prime} = 0\,; \tag{1}$$

the integration of (1) from x_L to x_R, making use of the new notation

$$C^\star(x,t) = \int_0^x c^\star(\xi, t)\mathrm{d}\xi\,,$$

then yields

$$\dot{C}^\star(x_R) - \dot{C}^\star(x_L) - v(c^\star(x_R) - c^\star(x_L)) = 0\,. \tag{2}$$

In the second section of this paper we shall sketch the physical background of the diffusive and massive phase transformation, applying the Onsager arguments. In the third section the derived system of equations for an unknown field c (because both j and v can be identified with certain functions of c) will be analyzed with the

aim to construct an effective algorithm searching for its approximate solution. The fourth section will demonstrate new numerical results for a special Fe-rich 3-component Fe-Cr-Ni alloy. The last section is reserved for concluding remarks and possible generalizations in several directions.

2. Physical background

Let us consider a closed system with the simple geometry, introduced above. Every index in all following relations can be understood as a sum index in sense of the Einstein rule; only an underlined index prohibits summation. Let i be an arbitrary index from $1, \ldots, q + r$ and f an arbitrary index from $\{\alpha, \beta, \gamma\}$ The chemical potential $\mu_i(x, c^\star)$ can be evaluated at every point of the sample as

$$\mu_i(x, c^\star) = w^f(x)\mu_i^f(c^\star) \,, \tag{3}$$

making use of some reasonably continuous weight functions $w^f(x)$, having the properties

$$\begin{array}{llll}
w^\alpha(x) = 1 \,, & w^\gamma(x) = 0 & \text{if} & x_L < x < h/2 \,, \\
w^\alpha(x) = 0 \,, & w^\gamma(x) = 1 & \text{if} & h/2 < x < x_R \,, \\
w^\beta(x) = 1 - w^\alpha(x) - w^\gamma(x) & \text{if} & x_L < x < x_R \,.
\end{array}$$

The well-known Gibbs-Duhem relation, formulated e.g. in [9], yields

$$c_i \frac{\mathrm{d}\mu_i^f}{\mathrm{d}t} = 0 \,, \qquad c_i \mu_i^{f\prime} = 0 \,. \tag{4}$$

The total Gibbs energy of the system is given by

$$G = \frac{1}{\Omega} \int_{x_L}^{x_R} c_i \mu_i \, \mathrm{d}x \,.$$

Its time derivative can be expressed as

$$\frac{\mathrm{d}G}{\mathrm{d}t} = \frac{1}{\Omega} \int_{x_L}^{x_R} \left(\frac{\mathrm{d}c_i}{\mathrm{d}t} \mu_i + c_i \frac{\mathrm{d}\mu_i}{\mathrm{d}t} \right) \mathrm{d}x \,.$$

Inserting μ_i into the second additive term from (3) and integrating by parts, we obtain

$$\mathrm{d}G/\mathrm{d}t = \frac{1}{\Omega} \int_{x_L}^{x_R} \left(\mathrm{d}c_i/\mathrm{d}t \, \mu_i + c_i w^f \mathrm{d}\mu_i^f/\mathrm{d}t - v c_i (w^f \mu_i^f)' + v c_i w^f \mu_i^{f\prime} \right) \mathrm{d}x \,.$$

By (4) the second and fourth additive terms vanish, moreover $w^f = 1$ for any $f \in \{\alpha, \gamma\}$ if $x \leq 0$ or $x \geq h$, thus we come to the result

$$\mathrm{d}G/\mathrm{d}t = \frac{1}{\Omega} \int_{x_L}^{x_R} \mathrm{d}c_i/\mathrm{d}t \, \mu_i \, \mathrm{d}x - \frac{v}{\Omega} \int_0^h c_i \mu_i' \, \mathrm{d}x \,.$$

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By (1), integrating by parts for a closed system again, we have finally

$$dG/dt = \int_{x_L}^{x_R} j_i \mu'_i \, dx - \frac{v}{\Omega} \int_0^h c_i \mu'_i \, dx \,. \tag{5}$$

The rate of dissipation Q of the total Gibbs energy can be evaluated by [13] in the form

$$Q = \int_{x_L}^{x_R} \frac{j_i^2}{A_i} \, dx + \frac{v^2}{M} \tag{6}$$

where

$$A_i = \frac{c_i D_i}{\Omega R T} \,, \tag{7}$$

D_i is the tracer diffusion coefficient, R is the gas constant, T is the absolute temperature and M is the interface mobility.

The kinetics of our system corresponds to the variation

$$\delta \left(dG/dt + \frac{Q}{2} \right) (j^\star, v) = 0$$

with respect to the above mentioned constraint for substitutional components: if k is an index similar to i, but from $\{1, \ldots, q\}$ only, then we can write

$$\delta \left(dG/dt + \frac{Q}{2} + \lambda \delta_{kk} \right) (j^\star, v, \lambda) = 0$$

with certain Lagrange multiplier λ, but without any additional constraints; all δ with a couple of indices, here and everywhere later, refer to Kronecker symbols. To support the brief notation, let us introduce the component type factor a_i, equal to 1 for $i \leq q$, zero otherwise. Performing the variation, step by step, for $j_1, \ldots, j_q, \ldots, j_{q+r}$, v and λ, we obtain

$$\int_{x_L}^{x_R} \left(\widetilde{j}_i \mu'_i + \frac{\widetilde{j}_i j_i}{A_i} + \widetilde{j}_i a_i \lambda \right) dx = 0$$

for every $\widetilde{j}_i$,

$$-\frac{\widetilde{v}}{\Omega} \int_0^h c_i \mu'_i \, dx + \frac{\widetilde{v} \, v}{M} = 0$$

for every $\widetilde{v}$ and formally also $\widetilde{\lambda} j_i a_i = 0$ for every $\widetilde{\lambda}$. In this way we come to $q + r$ differential equations

$$\mu'_i + \frac{j_i}{A_i} + \lambda a_i = 0 \tag{8}$$

with a parameter λ for all both substitutional and interstitial components and to one integral equation

$$v = \frac{\Omega}{M} \int_0^h c_i \mu'_i \, dx \tag{9}$$

for the interface velocity. It is not difficult to remove λ from (8): multiplying (8) by A_i and summing results with non-zero a_i, we have

$$\delta_{kk}A_k\lambda = -A_k\mu'_k - \delta_{kk}j_k = -A_k\mu'_k$$

and consequently

$$\lambda = -\frac{A_k\mu'_k}{\delta_{ll}A_l}$$

where l is a sum index with the same properties as k. This enables us to evaluate all fluxes as

$$j_i = -A_i\left(\mu'_i - a_i\frac{A_k\mu'_k}{\delta_{ll}A_l}\right);\tag{10}$$

let us notice that we have

$$\delta_{kk}j_k = \delta_{ii}a_ij_i = 0$$

and consequently the system of $q + r$ equations (8) can be reduced to the system of $q - 1 + r$ equations.

For practical calculations we need to express j_i by means of (10), (7) and (3); it is useful to introduce the decomposition

$$\mu^f_i(c^\star) = \mu^f_{0i} + RT\ln c_i + \varphi^f_i(c^\star)\tag{11}$$

where μ^f_{0i} are constants for a given temperature T and φ^f_i are certain functions of $c^\star$ (usually not dominant, but non-negligible and formally complicated). Inserting this decomposition together with (10) into (8), after rather long calculations, performed in [15], p. 75, we are able to evaluate

$$N\Omega j = -Bc' - Kc\tag{12}$$

where B, K (functions of c) and N (dependent on x only) are square matrices of order $q - 1 + r$, B full one, K and N diagonal ones, of the following material characteristics:

$$B_{mn} = \delta_{mn} + \frac{c_m(\zeta_q - \zeta_n)}{\eta} + \frac{\overline{\varphi}_{mn} - \overline{\varphi}_{mn}}{RT}, \qquad K_{\underline{mm}} = \frac{\overline{\mu}_m}{RT}, \qquad N_{\underline{mm}} = \frac{1}{\zeta_mD};$$

here m or n refer (instead of i) to a sum index from $\{1,\ldots,r-1,q+1,\ldots,q+r\}$ and moreover $\zeta_i = D_i/D$ for some (non-zero) reference value D of the tracer diffusion coefficient, $\eta = \zeta_ic_i$ and

$$\overline{\varphi}_{mn} = \widehat{\varphi}_{mn} - a_ma_n\frac{\zeta_lc_l}{\eta}\widehat{\varphi}_{ln}, \qquad \overline{\mu}_m = \widehat{\mu}_m - a_m\frac{\zeta_lc_l}{\eta}\widehat{\mu}_l$$

with $\widehat{\mu}_m = w^{f\prime}\left(\mu^f_{0m} + \varphi^f_m\right)$ and $\widehat{\varphi}_{mn} = w^f\partial\varphi^f_m/\partial c_n$. For any variable u let us introduce the simplified notation $u^\diamond = u(0)$, $u^L = u(x_L)$ and $u^R = u(x_R)$. Then, integrating (1) from 0 to x, omitting c_q and j_q, we receive

$$\dot{C} - v(c - c^\diamond) + \Omega(j - j^\diamond) = 0.\tag{13}$$

In particular, subtracting (13) with $x = x_R$ and $x = x_L$,

$$\dot{C}^R - v(c^R - c^\diamond) - \Omega j^\diamond = 0 , \qquad \dot{C}^L - v(c^L - c^\diamond) - \Omega j^\diamond = 0 , \tag{14}$$

we have only a formal modification of (2)

$$\dot{C}^R - \dot{C}^L - v(c^R - c^L) = 0 , \tag{15}$$

but inserting (12) into (13), we obtain a new result

$$-N\dot{C} + Bc' + (K + vN)c = vNc^\diamond - N\Omega j^\diamond . \tag{16}$$

3. Mathematical formulation and computational algorithms

We suppose that all values of molar fractions c are prescribed for $t = 0$. For their initial time derivatives we usually have no better information than $\dot{c} = 0$, thus also $\dot{C} = 0$ and $j^\diamond = 0$ from (14). Let us also notice that C can be computed as integrals of $c - c^a$ instead of c, using arbitrary reference constant admissible molar fractions c^a. Our problem is to find c from (16) with v inserted from (9). For a priori known B, K and v and also x_L, to solve (16) numerically (to construct a sequence of approximate solutions, whose limit could be expected to coincide with the solution of (16)) means to discretize (16) in time; this can be done by means of the Euler implicit scheme

$$Bc' + (K + vN)c - N\frac{C}{\tau} = vNc^\diamond - N\Omega j^\diamond - N\frac{C^\times}{\tau} \tag{17}$$

where τ denotes the time step and all variables are evaluated in time t, except $C^\times = C(t - \tau)$. (The application of more advanced schemes of discretization in time instead of (17) is possible, but leads to rather complicated forms of following equations.) To obtain a system of linear algebraic equations, we have to apply the discretization in $\langle x_L, x_R \rangle$, too. In practice only some estimates of all material characteristics B and K, of the interface velocity v and of the boundary position x_L (then clearly $x_R = x_L + H$) are available, usually those from the previous time step, thus (17) forms a basis for an iteration procedure where v can be recalculated from (9) using the Simpson rule; also the evaluation of C needs some numerical integration.

Let us consider a sufficiently large fixed interval $\mathcal{I}$, containing $\langle x_L, x_R \rangle$, decomposed to a finite number σ of subintervals $\langle x_{s-1}, x_s \rangle$, using $\sigma + 1$ nodes $x_0, x_1, \ldots, x_\sigma$. Then we can write (17) in the form

$$\overline{B}^s \frac{c^s}{\Delta_s} + \left(\overline{K}^s + v\overline{N}^s\right) \frac{c^s}{2} - \overline{N}^s \frac{\Delta_s c^s}{2\tau} \tag{18}$$

$$= \overline{B}^s \frac{c^{s-1}}{\Delta_s} - \left(\overline{K}^s + v\overline{N}^s\right) \frac{c^{s-1}}{2} + v\overline{N}^s c^\diamond - \overline{N}^s \Omega j^\diamond - \overline{N}^s \frac{2(C^{\times s} - C'^{s-1}) - \Delta_s c^{s-1}}{2\tau}$$

where an integer s refers to the s-th node in $\mathcal{I}$ (values at x_L and x_R, in general not identical with any x_s, are interpolated), $\Delta_s = x_s - x_{s-1}$ and overlined s-indexed symbols refer to averaged values on $\langle x_{s-1}, x_s \rangle$. Let us notice that $c^\diamond$ coincides always with

some element of the set $\{c^0, c^1, \ldots, c^\sigma\}$. Our aim is to study the long-time behaviour of a system, thus it is useful to take sufficiently small Δ_s in comparison with τ. We would like to solve $c^0, c^1, \ldots, c^s, \ldots$ effectively, step by step, but this is impossible because of unknown values $c^\diamond$ and $j^\diamond$ (the system of linear algebraic equation is not triangular). However, we shall show that this difficulty can be overcome: the main idea will be demonstrated on (17), its formal implementation into (18) will be left to the reader. Let $c^{\diamond e}$ be some estimate of $c^\diamond$ (from the preceding iteration, if not available yet then from the previous time step). Let us consider $c_m^\diamond = \xi_{\underline{m}}^I c_m^{\diamond e}$ and $j_m^\diamond = \xi_{\underline{m}}^{II} v c_m^{\diamond e}$ for some positive real $2(q-1+r)$ factors ξ_m^I and ξ_m^{II}. We are allowed to seek for molar fractions c in the form $c = c^\diamond + \widetilde{c}$ where $\widetilde{c}_m = \widetilde{c}_m^O + \xi_{\underline{m}}^I \widetilde{c}_m^I + \xi_{\underline{m}}^{II} \widetilde{c}_m^{II}$. Then (17) degenerates to

$$B\widetilde{c}' + K\widetilde{c} + vN\widetilde{c} - N\frac{\widetilde{C}}{\tau} = F^O + \xi_I F^I + \xi_{II} F^{II}$$

with $\widetilde{C}$ integrated from $\widetilde{c}$ (for comparison: C is integrated from $c - c^a$) and with

$$F^O = N\frac{C^\times - c^a x}{\tau}, \qquad F^I = \left(N\frac{x}{\tau} - K\right) c^{\diamond e}, \qquad F^{II} = -N\Omega v c^{\diamond e}.$$

Thus we are able to solve all $\widetilde{c}^O$, $\widetilde{c}^I$ and $\widetilde{c}^{II}$ separately (which is very simple) and just at the end to calculate ξ^I and ξ^{II} $(q-1+r)$-times from the system of two linear algebraic equations

$$\begin{bmatrix} \widetilde{C}_m^{LI}/\tau - v\widetilde{c}_m^{LI} + c_m^{\diamond e} x_L/\tau & \widetilde{C}_m^{LII}/\tau - v\widetilde{c}_m^{LII} \\ \widetilde{C}_m^{RI}/\tau - v\widetilde{c}_m^{RI} + c_m^{\diamond e} x_R/\tau & \widetilde{C}_m^{RII}/\tau - v\widetilde{c}_m^{RII} \end{bmatrix} \cdot \begin{bmatrix} \xi_m^I \\ \xi_m^{II} \end{bmatrix} =$$

$$\begin{bmatrix} -\widetilde{C}_m^{LO}/\tau + v\widetilde{c}_m^{LO} + C_m^{L\times}/\tau + c_m^a x_L/\tau \\ -\widetilde{C}_m^{RO}/\tau + v\widetilde{c}_m^{RO} + C_m^{R\times}/\tau + c_m^a x_R/\tau \end{bmatrix}.$$

The above sketched algorithm have been tested with the support of standard MATLAB environment. No special packages were needed, except the toolbox *symbolic*, referring to the core of MAPLE. Typically the material description for one calculation, generated for a fixed temperature of phase transformation, contain thousands of instructions; the most complicated are the expressions for chemical potentials in particular phases, especially their nonlinear parts, occurring as the last additive terms in the decomposition (11). Open questions are both in the theory of existence of solutions c and v and in the convergence of all algorithms. Some modifications of such algorithms, namely the application of higher-order Hermite splines (in the approximation of both unknown molar fractions and material characteristics) and of the spectral analysis in the phases α and γ, far from the interface, where nearly exponential distributions of molar fractions can be expected, are discussed in [15], p. 79.

The rather complicated non-local integro-differential character of the problem does not admit the application of some transparent homogenization technique. Moreover, the identification of material characteristics, included in B, K and N, is very

complicated; consequently it is not clear how to formulate and study the inverse problems (formulation of all chemical potentials and diffusion factors, generating B, K and N, and setting the interface mobility M, the interface thickness h, etc., from experimental results for $c(x, t)$ at some set of fixed guaranteed temperatures) correctly. Most material characteristics can be classified as a semi-empirical ones, based both on some physical considerations and on the extensive experimental study, unfortunately not covering all mole fractions of particular components between 0 and 1. Moreover no physical barrier is incorporated into our system of equations to prevent negative or other non-realistic mole fractions; very different quantitative values of some characteristics, namely of the interface mobility M, can be found in the literature, too.

4. Numerical example

The numerical example, presented in this paper, makes use of the same source of quantitative material data as [14] from the Montanuniversität Leoben (Austria) and from the Institute of Physics of Materials of the Czech Academy of Sciences in Brno. We have the purely substitutional three-component Fe-Cr-Ni system; in our notation $q = 3$ and $r = 0$, moreover Fe will be dominant.

The tracer diffusion coefficients can be interpolated using the formula

$$\ln D_k = w^f \ln D_k^f \ ,$$

thus it is sufficient to set nine values D_k^f. In general we have

$$D_k^f = D_{k0}^f \exp\left(-\frac{E^f}{RT}\right) \ , \qquad M = M_0 \exp\left(-\frac{E^\star}{RT}\right) \ .$$

The applied constants are for Cr (corresponding to $k = 1$) $D_{10}^\alpha = 0.00032$ m^2 s^{-2}, $D_{10}^\beta = 0.00022$ m^2 s^{-2}, $D_{10}^\gamma = 0.00035$ m^2 s^{-2}, for Ni ($k = 2$) $D_{20}^\alpha = 0.000048$ m^2 s^{-2}, $D_{20}^\beta = 0.000022$ m^2 s^{-2}, $D_{20}^\gamma = 0.000035$ m^2 s^{-2}, for Fe ($k = 3$) $D_{30}^\alpha = 0.00016$ m^2 s^{-2}, $D_{30}^\beta = 0.00011$ m^2 s^{-2}, $D_{30}^\gamma = 0.00007$ m^2 s^{-2}, and for all components $E^\alpha = 240000$ J mol^{-1}, $E^\beta = 155000$ J mol^{-1}, $E^\gamma = 286000$ J mol^{-1}, $E^\star = 140000$ J mol^{-1}; it remains to set only $M_0 = 0.00041$ m^2 s kg^{-1}.

Three figures show the time-variable distributions of c_1 and c_2. The interface thickness is $h = 5 \cdot 10^{-10}$ m, the sample length $H = 10^{-4}$ m. From the originally constant mole fractions $c_1 = 0.001$ and $c_2 = 0.019$ (consequently $c_3 = 0.980$) in all phases due to the phase transformation driven by changes in chemical potentials, the time development from $t = 0$ to $t = 70000$ s leads to qualitative new distributions. All figures make use of the same computational results at various scales: Fig. 1 shows Cr and Ni (strongly nonlinear) mole fractions inside the interface, Fig. 2 documents different behaviour of Cr and Ni components near the interface, Fig. 3 demonstrates quasi-constant distributions with seemingly sharp interface, whose physically transparent macroscopic description is not available. The numbers of particular curves from $\{1, \ldots, 7\}$ (quite omitted in Fig. 1, somewhere hardly recognizable even for larger scales) refer to $t \in \{10000, \ldots, 70000\}$ s.
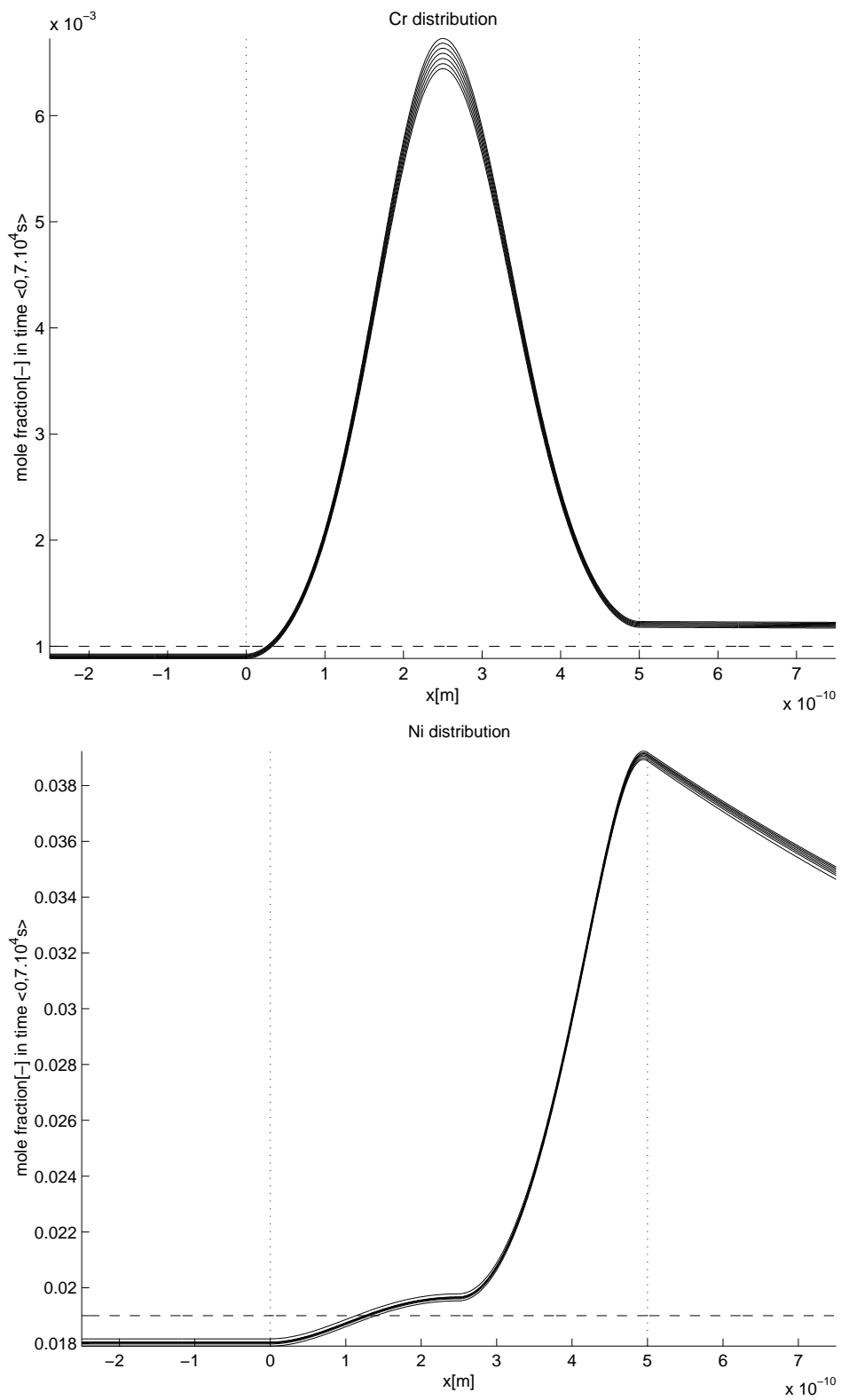
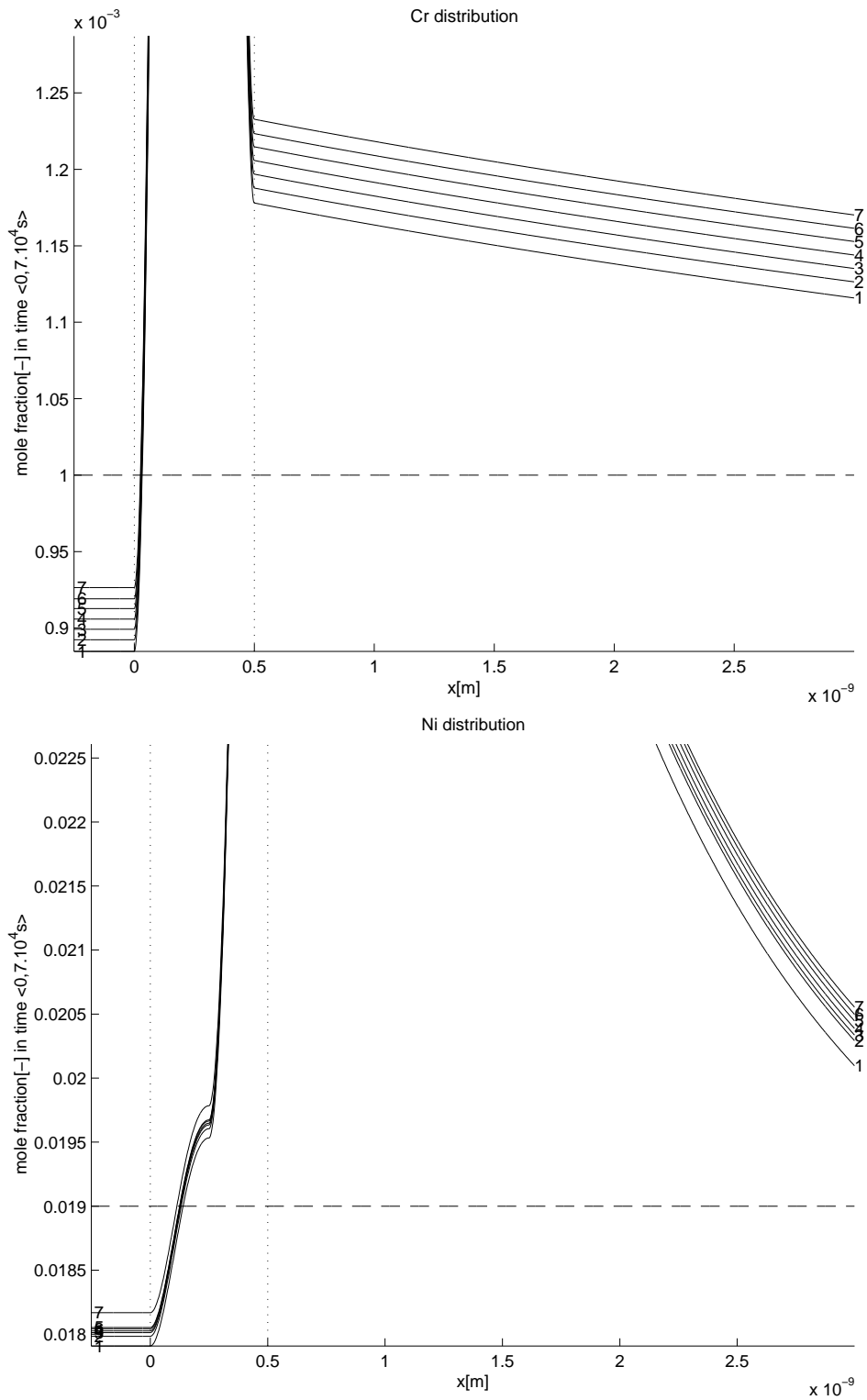**Fig. 1:** *Nano-scale distribution of Cr and Ni inside the interface.*

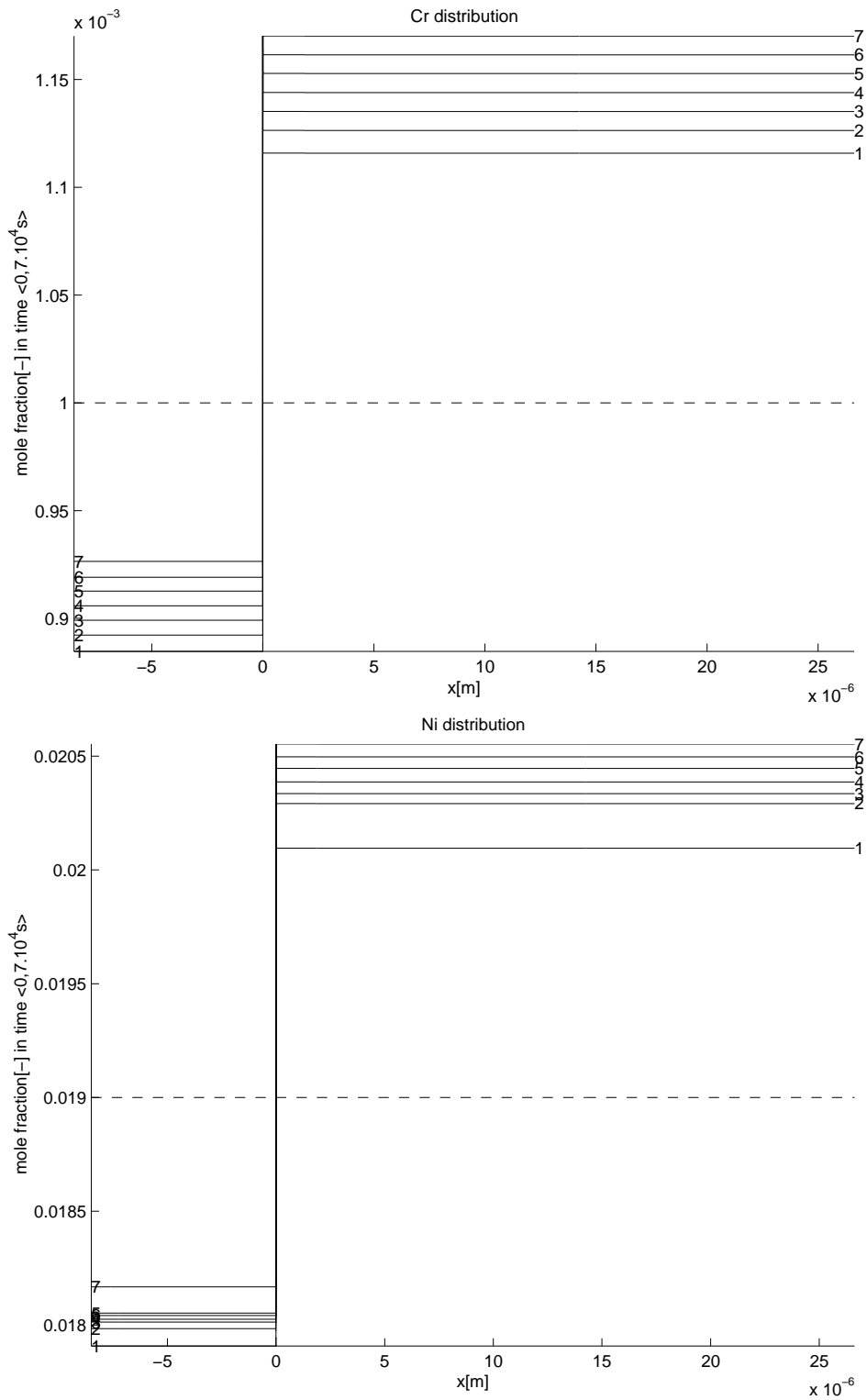**Fig. 2:** *Meso-scale distribution of Cr and Ni near the interface.*

Fig. 3: *Larger-scale observable distribution of Cr and Ni.*

5. Conclusions and generalizations

In our numerical example we have seen the typical non-stationary behaviour of one special Fe-rich Fe-Cr-Ni substitutional system, described by (16) and (9), with respect to the physical limitations (a finite closed system, interface of constant thickness, substitutional components). However, the created software has been tested for more classes of problems of practical importance. In [14] the stationary solver was applied to the Fe-rich Fe-Cr-Ni substitutional system with various types of chemical potentials and values of material characteristics, which may be rather uncertain in practice, namely in case of the interface mobility and thickness; further numerical simulations has been done also for the similar system with the interstitial C-component and for the binary Al-Mg system yet. For every fixed interface thickness h the numerical simulations show that the interface velocity v decreases with the increasing temperature T; finally the phase transformation stops at certain critical temperature. This critical temperature increases with the increasing interface thickness h; the limit case $h \to 0$ returns the (less realistic) results for an idealized sharp interface. The simulation of the massive $\gamma \to \alpha$ transformation shows that the existence of the solute drag in the interface influences the contact conditions at the interface allowing the massive transformation to occur also in the two-phase region. By choosing α and γ as identical phases and by imposing fluxes to the interface (grain boundary), diffusion induced grain boundary motion was simulated. The interface and grain boundary Gibbs energy were calculated; their realistic values support the responsibility of the model.

Both theoretical and experimental works yield that the diffusion in multi-component alloys can be characterized by three attributes: a) the vacancy mechanism for "slowly" diffusing substitutional components, b) the existence of certain sources or sinks of vacancies, c) the "quick" motion of atoms of interstitial components. In our description only the attributes a) and c) have been incorporated properly; the attribute b) should be involved using the detailed analysis [11], referring to [3]. Another important research direction is to admit more complicated thermal processes. This forces (from the point of view of the Onsager relation) coupling of various fluxes, namely the particle flux due to a temperature gradient (Soret effect) and the transport of heat due to a concentration gradient (Dufour effect); more information is contained in [12]. Still another direction of possible generalizations leads to two- or three-dimensional simulations. Up to now, such computations suffer from the lack of reasonable material data; nevertheless, an introductory discussion is included in [15], p. 85.

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