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SCALE BRIDGING IN DIFFUSIVE PHASE TRANSFORMATION [*]

JIŘÍ VALA [†]

Abstract. The physical micro- and nano-scale analysis of phase transformation of materials consisting of a finite number of substitutional and interstitial components, based on the Onsager extremal thermodynamic principle, leads to a system of partial differential equations of evolution type containing certain integral term, whose form differs substantially in both phases and in the moving phase interface of finite thickness, in whose center the ideal liquid material behaviour can be detected. Even in the case of a model one-dimensional problem at certain fixed temperature, unlike e. g. the classical problems of thermal transfer, no reasonable macro-scale equations, working with "effective" material characteristics as results of some formal homogenization procedure, are available. However, the reliable evaluation both of the velocity of phase transformation and of all distributions of concentrations (or molar fractions) of particular components is needed. This paper offers a possibility of an indirect effective computational prediction of such process of diffusive and massive transformation, making use of the large database of micro-scale material properties and of the MATLAB-supported simulations, applicable even for very complicated evaluations of chemical potentials and diffusion factors.

Key words. Micro- and nano-scale computational modelling, non-stationary diffusive and massive phase transformation, multi-component systems, thermodynamic principles, integro-differential problems, finite difference method, method of discretization in time, MATLAB-supported simulations.

AMS subject classifications. 74N25, 74N15, 74S20.

1. Introduction. Most models of diffusional phase transformation, involving bulk diffusion and interface migration, pay attention especially to binary (two-component) alloys with substitutional components – cf. [3] and [10]. However, in practice the analysis of more general alloys with a finite number of q substitutional and r interstitial components is needed. In such cases usually the interface is idealized to be sharp (of negligible thickness), 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 [14]. However, a real migrating interface of a 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 [15], following some ideas of [12], coming from the Onsager extremal thermodynamic principle, formulated at the nano- or micro-scale level (the realistic value of h is 10^{-9}m), derived originally in [11] (for more details and various generalizations see [9]), the steady-state diffusion of solute across the interface is driven by the difference of chemical potentials $\mu(c)$, corresponding to the vector c of molar fractions (as concentrations characteristics) related to the first $q-1$ substitutional components, i. e. $c = (c_1, \ldots, c_{q-1})$; in this case we can evaluate the last molar fraction as $c_q = 1 - c_1 - \ldots - c_{q-1}$. As discussed in [6], at least for the steady-state case this approach gives identical results with the solute drag formula proposed

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[†] Department of Mathematics and Descriptive Geometry, Faculty of Civil Engineering, Brno University of Technology, 602 00 Brno, Veveří 95 (`vala.j@fce.vutbr.cz`).

in [8]. In [19] the same approach is generalized to admit the evolution of all molar fractions in time and the presence of r interstitial components; consequently $c = (c_1, \dots, c_{q-1}, c_{q+1}, \dots, c_{q+r})$. Nevertheless, [19] shows only one practical example of such evolution near the initial time; the algorithm suggested in this paper handles also slow long-time redistributions.

Most multi-scale approaches try to perform the micro-scale computations at certain (sufficiently small) periodic or quasi-periodic representative volume element and to extend the results to the macro-scale (or, step-by-step, to the meso- and macro-scale) analysis, using some artificially homogenized ("effective") material characteristics. Nevertheless, the required mathematical techniques are often unfriendly to physicists or material, civil, mechanical, etc. engineers: e.g. the existence and convergence results of the two-scale homogenization for the standard problem of heat transfer in materials with a fully periodic material structures, formulated in [1], p. 204, and similar ones for the wave equations, for the linearized elastricity, etc., cannot be easily extended to more general structures (the classical calculus in the Lebesque and Sobolev spaces must be replaced by the deep results of functional analysis of Banach algebras or by the implementation of special probabilistic measures – cf. [4] and [5]). Moreover, the convergence analysis of numerical algorithms comes typically from the arguments based on the generalized Cauchy-Schwarz inequality, assuming some scalar products in Hilbert spaces (for the details see [20]), not available for general formulations. Therefore it is difficult to reject some critical opinions: e. g. [2] comments the multi-scale approach that "it begins with naive euphoria" and consequently there is an "overreaction to ideas that are not fully developed, and this inevitably leads to a crash". Even the approach applied in this paper is not able to construct any macro-scale limits directly; however, its nano- and micro-scale simulation can predict the global behaviour of the process of phase transformation in terms of observable quantities, as interface velocity and molar fractions of particular components. Some open questions and possible generalizations will be mentioned in the concluding section.

2. Physical background. Let us start with the geometrical description of the one-dimensional system. The evolution of $q - 1 + r$ molar fractions c is characterized in a Cartesian coordinate x and in time t. The coordinate x moves from the left to the right together with the interface of some constant thickness h (from $x = 0$ to $x = h$); the total size of the specimen is H (in practice much greater than h), the system is assumed to be closed (with zero boundary fluxes) on the interval $\langle x^L(t), x^R(t) \rangle$. For certain material sample of length H, in addition to c it is useful to introduce diffusive fluxes $j_1, \dots, j_{q+r}$ and their vector $j = (j_1, \dots, j_{q-1}, j_{q+1}, \dots, j_{q+r})$ where $j_1 + \dots + j_q = 0$. We are allowed to study the redistribution of c and j in an arbitrary positive time t with $j(.) = 0$ at the boundary (consisting of two points, whose distance is H). In such system we need only to know all initial values c for $t = 0$; no additional boundary conditions are needed. 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 $0 \le x \le h$.

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 ($\Omega c_1, \dots, \Omega c_{q+r}$ are just the concentrations of particular components) reads

$$\mathrm{d}c/\mathrm{d}t + \Omega j' = \dot{c} - vc' + \Omega j' = 0\,; \tag{2.1}$$

the integration of (2.1) from x^L to x^R, making use of the new notation

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

then yields

$$\dot{C}(x^R) - \dot{C}(x^L) - v(c(x^R) - c(x^L)) = 0\,. \tag{2.2}$$

The proper physical analysis of the diffusive and massive phase transformation comes from the thermodynamic Onsager principle; all details can be found in [18] (for the stationary case) and in [19] (for the non-stationary one). The total Gibbs energy of the system (with respect to the Gibbs-Duhem condition, formulated e. g. in [13]) is given by

$$G = \frac{1}{\Omega}\int_{x^L}^{x^R} c_i\mu_i\,\mathrm{d}x\,;$$

i here means the sum index from $\{1, \dots, q+r\}$) applied in sense of the Einstein rule (the underline symbol will prohibit the summing without any comments). Its time derivative can be expressed as

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

Each chemical potential $\mu_i(x,c)$ can be evaluated at every point of the specimen as

$$\mu_i(x,c) = w^f(x)\mu_i^f(c)\,, \tag{2.3}$$

making use of certain continuous weight functions $w^f(x)$ with the sum index $f \in \{\alpha,\beta,\gamma\}$, having the properties

$$\begin{array}{lll} w^\alpha(x) = 1\,, \quad w^\gamma(x) = 0 & \text{if} & x^L < x < h/2\,,\\ w^\alpha(x) = 0\,, \quad w^\gamma(x) = 1 & \text{if} & h/2 < x < x^R\,,\\ w^\beta(x) = 1 - w^\alpha(x) - w^\gamma(x) & \text{if} & x^L < x < x^R\,, \end{array}$$

and chemical potentials for particular phases $\mu_i^f(c)$, received from the experimental research. Consequently, integrating by parts, we obtain

$$\frac{\mathrm{d}G}{\mathrm{d}t} = \int_{x^L}^{x^R} j_i\mu_i'\,\mathrm{d}x - \frac{v}{\Omega}\int_0^h c_i\mu_i'\,\mathrm{d}x\,.$$

The rate of dissipation Q of the total Gibbs energy can be evaluated by [17] in the form

$$Q = \int_{x^L}^{x^R} \frac{j_i^2}{A_i}\,\mathrm{d}x + \frac{v^2}{M}$$

where

$$A_i = \frac{c_i D_i}{\Omega RT}\,, \tag{2.4}$$

D_i is the tracer diffusion coefficient, R is the gas constant, T is the absolute temperature (assumed as constant here) and M is the interface mobility.

The kinetics of our closed system can be characterized by the zero variation of a functional

$$\Phi = \left(\frac{\mathrm{d}G}{\mathrm{d}t} + \frac{Q}{2}\right)(j,v)\,.$$

Performing long computations, forcing the above mentioned constraint for substitutional components by one Lagrange multiplier, from the minimization of Φ we finally receive the system of equations of evolution

$$Bc' + (K + vN)c - N\dot{C} = vNc^\diamond - N\Omega j^\diamond \tag{2.5}$$

where all variables are evaluated in time t except $C^\times = C(t-\tau)$, B, K and N are square matrices of order $q-1+r$, B full, K and N diagonal, B and K depending on c, N dependent on x only, Ω is the constant molar volume and

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

$c^\diamond$ refers to molar fractions and $j^\diamond$ to diffusive fluxes at $x = 0$ and

$$v = \frac{\Omega}{M}\sum_{i=1}^{q+r}\int_0^h c_i\mu_i'\,\mathrm{d}x \tag{2.6}$$

for prescribed chemical potentials μ_i, decomposed by (2.3), as very complicated functions of c. The complete (not very reader-friendly) formulae for the evaluation of $B(c)$, $K(c)$ and $N(x)$ in terms of the phase chemical potentials μ_i^f and their derivatives can be found in ([19]); the evaluation of μ_i^f (even for the fixed T) for concrete systems needs MAPLE-supported pre-processing.

3. Mathematical formulation and computational modelling. The resulting system (2.5), starting from some a priori known initial values of c, can be rewritten in the form

$$Bc' + (K + vN)c - N\frac{C}{\tau} = vNc^\diamond - N\Omega j^\diamond - N\frac{C^\times}{\tau}\,; \tag{3.1}$$

τ denotes the time interval, referring to the implicit Euler method ((2.5) comes from the limit passage $\tau \to 0$). Let us notice that another consequence of (2.1) is

$$(C^R - C^{R\times})/\tau - v(c^R - c^\diamond) = (C^L - C^{L\times})/\tau - v(c^L - c^\diamond) = \Omega j^\diamond\,; \tag{3.2}$$

upper indices ^{L} and ^{R} here refer (for the simplicity of notation) to the values at x^L and x^R, respectively. Since (3.1) can generate an iterative procedure with B, K, v and x^L set by c from the preceding iteration (or time step), it is important to suggest an inexpensive solver of the system of linear algebraic equations, derived from (3.1), using the finite difference method. Unfortunately, such system is not triangular, thus, because of the presence of unknowns $c^\diamond$ and $j^\diamond$ it is not possible to express c in all nodes step-by-step; even $c^\diamond$ and $j^\diamond$ cannot be determined by (3.2) completely.

Let us 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 (3.1) with v inserted from (2.6). Clearly (3.1) requires some discretization in x, e. g. that using the finite difference technique again, whereas v from (2.6) needs the numerical integration, e. g. by the Simpson rule, and the same is true for C (which can be computed from integrals of $c - c^a$ instead of c, using arbitrary reference constant admissible molar fractions c^a). However, for simplicity we shall explain the main idea of the computational algorithm using the original semi-discretized system (3.1).

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 $c^\diamond_m = \xi^I_m c^{\diamond e}_m$ and $j^\diamond_m = \xi^{II}_m v c^{\diamond e}_m$ for some positive real $2(q-1+r)$ factors ξ^I_m and ξ^{II}_m; $m \in \{1, \dots, q-1+r\}$ are not sum indices. We are allowed to seek for molar fractions c in the form $c = c^\diamond + \widetilde{c}$ where $\widetilde{c}_m = \widetilde{c}^O_m + \xi^I_m \widetilde{c}^I_m + \xi^{II}_m \widetilde{c}^{II}_m$. Then (3.1) 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 $\widetilde{c}$, unlike C integrated from $c - c^a$ in general, and with

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

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

$$\begin{bmatrix} \widetilde{C}^{LI}_m/\tau - v\widetilde{c}^{LI}_m + c^{\diamond e}_m x^L/\tau & \widetilde{C}^{LII}_m/\tau - v\widetilde{c}^{LII}_m \\ \widetilde{C}^{RI}_m/\tau - v\widetilde{c}^{RI}_m + c^{\diamond e}_m x^R/\tau & \widetilde{C}^{RII}_m/\tau - v\widetilde{c}^{RII}_m \end{bmatrix} \cdot \begin{bmatrix} \xi^I_m \\ \xi^{II}_m \end{bmatrix} = \begin{bmatrix} -\widetilde{C}^{LO}_m/\tau + v\widetilde{c}^{LO}_m + C^{L\times}_m/\tau + c^a_m x^L/\tau \\ -\widetilde{C}^{RO}_m/\tau + v\widetilde{c}^{RO}_m + C^{R\times}_m/\tau + c^a_m x^R/\tau \end{bmatrix}. \tag{3.3}$$

Now let us sketch the fully discretized algorithm, generating (in each time and iterative step) a system of $2(q-1+r)$ linear algebraic equations. Using the above explained tricks with parameters ξ^I and ξ^{II}, we have an inexpensive solver; this is very useful in situations where e. g. the algebraic expressions for evaluation of $\mu(c)$ contain thousands of instruction, preprocessed by MAPLE or toolbox *symbolic* from the MATLAB software package.

We can write (3.1) in the form

$$\overline{B}^s\,\frac{c^s}{\Delta_s} + \Bigl(\overline{K}^s + v\overline{N}^s\Bigr)\,\frac{c^s}{2} = -\overline{N}^s\,\frac{\Delta_s c^s}{2\tau} \tag{3.4}$$

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

where an integer s refers to the s-th node in a sufficiently large interval, decomposed to fixed subintervals $\langle x_{s-1}, x_s \rangle$ (not moving with the interface – 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 all overlined s-indexed symbols refer to averaged values on $\langle x_{s-1}, x_s \rangle$; let us notice that $c^\diamond$ coincides with c^s always for some s. Clearly such scheme forces 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, using three versions of right-hand sides again, and complete them a posteriori, after setting ξ^I and ξ^{II} and consequently $c^\diamond$ and $j^\diamond$.

The reformulation of (3.3) in the notation of (3.4) is important for the programmer; nevertheless, here must be left to the reader. The following simulation example makes use of this algorithm, applying the semi-empirical chemical potentials from the Montanuniversität Leoben (Austria) and from the Institute of Physics of Materials of the Czech Academy of Sciences in Brno. The idea of its iterative algorithm (implemented in the MATLAB environment) can be roughly sketched as follows:

1. read initial values c, x^L, x^R and set $t = 0$, $v = 0$,
2. increment t by τ, estimate $c^* = c^\times$ and $v^* = v^\times$,
3. integrate v from c^* (using the Simpson rule applied to 2.6), update x^L and x^R,
4. evaluate (in all nodes) $B(c^*)$, $K(c^*)$ and $N(x)$,
5. solve (step by step) $\widetilde{c}^\diamond$, $\widetilde{c}^I$ and $\widetilde{c}^{II}$ from (3.4), simultaneously $\widetilde{C}^\diamond$, $\widetilde{C}^I$ and $\widetilde{C}^{II}$,
6. determine parameters ξ^I and ξ^{II} and find c,
7. if error of $c - c^*$ or $v - v^*$ is not negligible, set $c^* = c$, $v^* = v$ and go back to 3.
8. if time limit is still not reached, set $c^\times = c$, $C^\times = C$, $v^\times = v$ and go back to 2.

4. Illustrative example. For the physical interpretation of all following material charcteristics let us refer to [18]. 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 from (2.4) D_i, $i \in \{1, 2, 3\}$, can be interpolated using the formula

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

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

$$D_i^f = D_{i0}^f \exp\left(-\frac{E^f}{RT}\right) \ , \qquad M = M_0 \exp\left(-\frac{E^\star}{RT}\right) \ .$$

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

Three figures show the couples of time-variable distributions of c_1 and c_2, corresponding to Cr (left graphs) and Ni (right ones). The time is varying from 0 to 70000 s; the dashed curves refer to the initial state, the curves numbered from 1 to 7

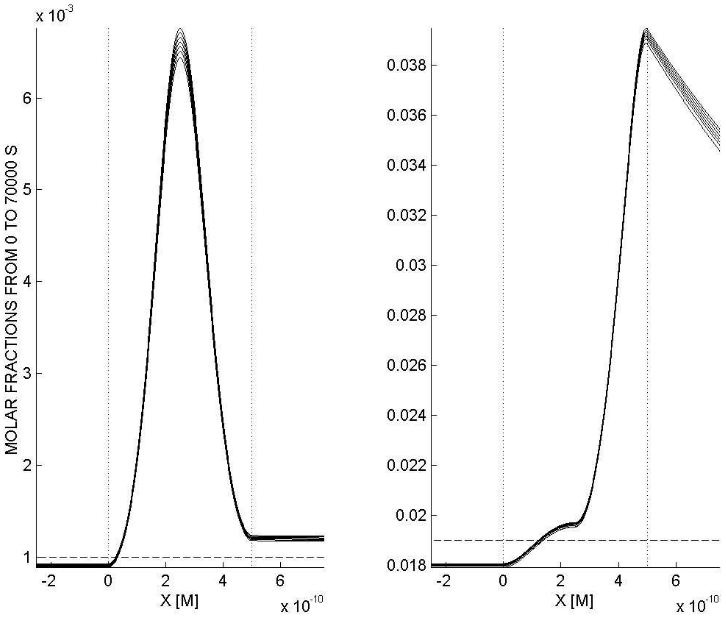

FIG. 4.1. *The time development of Cr and Ni molar fractions inside the interface*

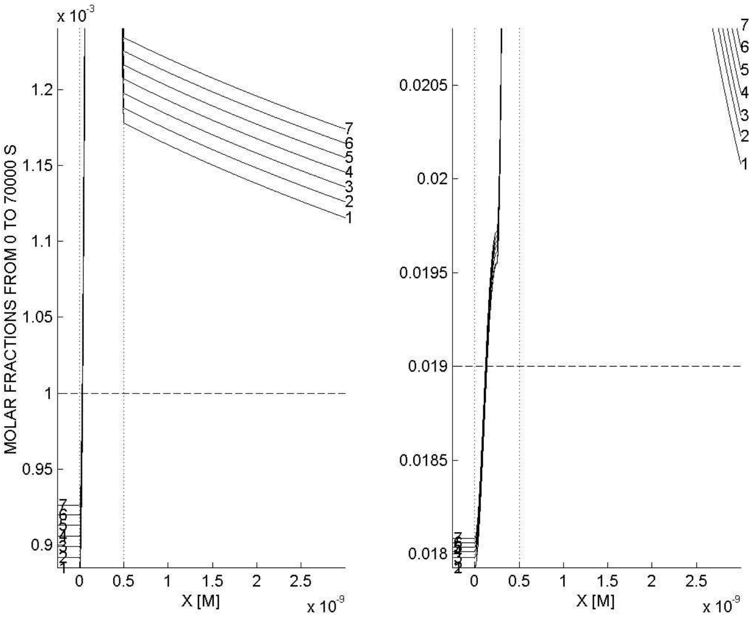

FIG. 4.2. *The time development of Cr and Ni molar fractions near the interface*

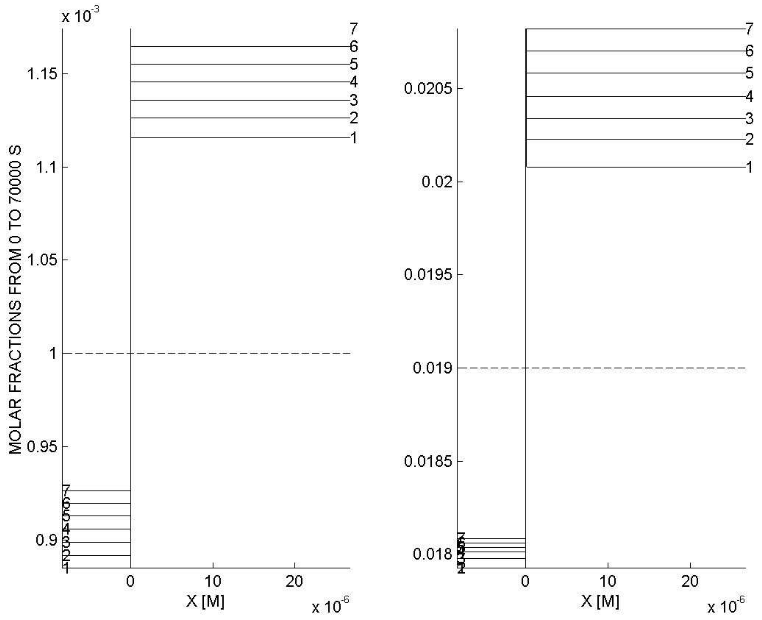

FIG. 4.3. *The time development of seemingly constant observable Cr and Ni molar fractions*

(these numbers are omitted at Fig. 4.1) correspond to $10000, 20000, \ldots 70000$ s. The interface thickness is $h = 0.5$ nm, the computational specimen length is $H = 0.1$ mm. The couple of dotted lines separate both the phases α and β, and the phases β and γ. From the originally constant molar 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 leads to qualitatively new distributions.

Fig. 4.1 presents the results of nano-scale (if classified in meters) computations inside and very close to the interface. We can see that no simple limit passage $h \to 0$ is available. Still other arguments for this statement can be found in [18]: e. g. even in the (quasi-)stationary case the decrease of v with growing T (expected by laboratory experiments and practical observations) is not quite independent of h, thus the idea of a sharp interface is unacceptable. Fig. 4.2 documents the larger-scale behaviour of molar fractions relatively near the interface. Fig. 4.3 shows a micro- (or slightly larger-) scale view here: nearly constant molar fractions, separated by a seemingly sharp interface, can be observed (but not completely explained from the simplified theory assuming a sharp interface).

5. Conclusions and generalizations. In the illustrative numerical example we have seen the typical non-stationary behaviour of one special Fe-rich Fe-Cr-Ni substitutional system, described by (3.1) and (2.6) (supplied by boundary and initial conditions), with respect to the physical limitations (a finite closed system, interface of constant thickness, substitutional components). The natural generalization of the introduced approach leads to the two- or three-dimensional simulations. However, such computations suffer from the lack of reasonable material data (which is a motivation for the development of advanced measurement techniques and identification algorithms); from other difficulties we can highlight the non-existence of integrals C, important in our one-dimensional approach (the finite element or finite volume techniques should be helpful here) and the variable position and curvature of the moving interface; more information is included in [19], p. 85.

The created software, covering (up to now) the one-dimensional problem, has been tested for more classes of problems of practical importance. In [18] 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 have been done also for the similar system with the interstitial C-component and for the binary Al-Mg system yet. We have noticed that for a fixed interface thickness h 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 growing interface thickness h; the limit case $h \rightarrow 0$ returns the (less realistic) results for an idealized sharp interface. The simulation of the massive $\gamma \rightarrow \alpha$ 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.

The remaining comments refer to the useful research for the near future. Both theoretical and experimental studies conclude that that the diffusion 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 this paper only the attributes a) and c) have been incorporated properly; the attribute b) should be involved using the detailed analysis [15], referring to [7]. Another important research direction is to admit more complicated thermal processes. This forces (from the point of view of the Onsager relation), following [16], 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). Still open questions are also in the theory of existence of solutions (the results of [10] cannot be easily extended to non-binary alloys), especially in the non-stationary case, and in the convergence of computational algorithms; such proper study is needed for the complete analysis at multiple scales, i. e. for the correct evaluation of the effect of various simplifications and homogenization attempts, not only of that classical with $h \rightarrow 0$.

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