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NUMERICAL MODELLING OF FE-CR-NI DIFFUSIVE PHASE TRANSFORMATION [*]

JIŘÍ VALA [†] AND JIŘÍ SVOBODA [‡]

Abstract. An original one-dimensional model for the diffusive phase transformation in substitutional alloys, based on the application of the Onsager thermodynamical extremal principle, is derived and applied to a Fe-rich Fe-Cr-Ni system. The model assumes the interface of finite thickness with finite mobility and solute segregation and drag in the migrating interface. One typical example of calculation of concentration profiles of Cr, Ni and Fe in two phases γ and α, where $\gamma \to \alpha$ transformation is active, and in their interface (in 3 variants) is presented in details; more results obtained by the same MATLAB-based simulation software are discussed.

Key words. Extremal principles in thermodynamics, diffusive phase transformation, massive phase transformation, numerical analysis of systems of ODEs.

AMS subject classifications. 74N25.

1. Introduction. The general overview of problems of diffusion in solids can be found in [2]. To simulate diffusional phase transformations it is necessary to solve the coupled problem of bulk diffusion and interface migration. Usually some ortho- or para-equilibrium contact conditions at the interface are applied. A more advanced approach is presented in [1]: it restricts the continuity in chemical potentials only to the interstitial elements (not to the substitutional ones). If no solute drug effects in the migrating interface (of the finite mobility) occur, the jumps of the substitutional elements can be derived from the Onsager thermodynamic extremal principle of maximum dissipation, using the access of [5]. Nevertheless, if such effects are not negligible, the jump conditions for corresponding chemical potentials change significantly.

In this contribution a model for massive transformation, taking into account the solute drag in the interface of finite thickness, will be derived and applied to the phase transformation of a Fe-rich Fe-Cr-Ni system: 0.1 % Cr and 1.9 % Ni will be set for simulation. Unlike the approach of [7] the system of differential equations will be formulated more carefully to avoid numerical instabilities even in case of rapid changes of diffusive coefficients on the interface between the α and γ phases and to handle complicated semi-empirical expressions for the evaluation of chemical potentials both in the α and γ phases, obtained on base of the extensive experimental work at the Montainuniverisität Leoben.

2. Physical background. We shall consider a closed one-dimensional system with 3 substitutional components, occuring in our Fe-Cr-Ni system. (In [7] the natural generalization to a finite number of components is considered, but this will not be necessary here.) Two phases, α and γ, will be separated by a migrating incoherent interface; the $\alpha \to \gamma$ transformation will be active. The local chemical composition is

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[†] Brno University of Technology, Faculty of Civil Engineering, Department of Mathematics and Descriptive Geometry, 602 00 Brno, Žižkova 17, Czech Republic (`vala.j@fce.vutbr.cz`)

[‡] Academy of Sciences of the Czech Republic, Institute of Physics of Materials, 616 62 Brno, Žižkova 22, Czech Republic (`svobj@ipm.cz`)

described by concentrations c_1, c_2 and c_3 for particular components in the following order: Cr, Ni and Fe (dominant, $c_3 = 1 - c_1 - c_2$). The chemical potentials μ_1, μ_2 and μ_3 depend both on c_1, c_2 and c_3 and on the coordinate x directly (for the details see below). The interface of the constant thickness is assumed to move from the left to the right. No deformation at any point due to diffusion or phase transformation, no sources or sinks of vacancies and no stresses in the system (consequently: no mechanical driving force for a coupled process of bulk diffusion and interface migration) will be included into the model.

More precisely, we shall make use of the following notation:

i component index ($i \in \{1, 2, 3\}$),
c_i component concentration,
j_i component diffusive flux,
x coordinate in the one-dimensional Euclidean space ($x \in \Omega = [0, H]$, H is a positive real constant),
t time coordinate ($t \in [0, \infty)$),
I position of moving interface ($I = [x_L(t), x_R(t)]$, $h = x_R(t) - x_L(t)$ is a positive real constant, independent of t, $h < H$),
v interface migration rate (constant on I, variable in time in general).

The Einstein summation rule (for repeated indices) will be preserved; if some index is underlined then the summation is not allowed. The indices i, k, l will be assumed to be from $\{1, 2, 3\}$ everywhere; δ will be reserved for the Kronecker symbol ($\delta_{ik} = 1$ for $i = k$, $\delta_{ik} = 0$ otherwise).

The material characteristics are three diffusive coefficients D_i, one interface mobility M and three chemical potentials μ_i. In the following considerations also the diffusive factor

$$A_i = c_{\underline{i}} D_i / (RT)$$

for the constant $R = 8314 \ \mathrm{J\,K^{-1}\,mol^{-1}}$ and for certain fixed temperature T will be useful. Moreover, λ is the Lagrange multiplier (forcing the "Kirchhoff law" $\delta_{ii} j_i = 0$). A prime symbol will denote a derivative by x, a dot symbol a (total) derivative by t briefly.

Usually the diffusive coefficients D_i^α and D_i^γ for the phases α and γ are known; the same is true for the diffusive coefficients D_i^β, corresponding to an ideal liquid state β of material. However, such diffusive coefficients D_i^β are correct just in the interface center $x_C = (x_L + x_R)/2$; the diffusive coefficients D_i inside the interface ($x_L < x < x_R$) have to be interpolated applying the formula

$$\ln D_i(x) = \xi_D^\alpha(x) \ln D_i^\alpha + \xi_D^\beta(x) \ln D_i^\beta + \xi_D^\gamma(x) \ln D_i^\gamma \,.$$

In this formula $\xi_D^\alpha(x)$, $\xi_D^\beta(x)$ and $\xi_D^\gamma(x)$ are such polynomial weight functions of order 4 that

$$D_i(x_L) = D_i^\alpha \,, \qquad D_i(x_R) = D_i^\gamma \,, \qquad D_i(x_C) = D_i^\beta \,, \qquad D_i'(x_L) = D_i'(x_R) = 0 \,.$$

The coefficients of all polynomials $\xi_D^\alpha(x)$, $\xi_D^\beta(x)$ and $\xi_D^\gamma(x)$ can be derived easily, using the Newton form of the Hermite interpolation scheme. We shall also use dimensionless factors $\zeta_i(x) = D_i(x)/D_3^\alpha$; then we shall write D instead of D_3^α briefly.

The formulation of 3 chemical potentials can be done in the similar way: we can distinguish

$$\mu_i(x, c) = \mu_{i0}(x) + RT(\ln c_i + \varphi(x, c))$$

where

$$\mu_{i0}(x) = \xi_\mu^\alpha(x)\mu_{i0}^\alpha + \xi_\mu^\beta(x)\mu_{i0}^\beta + \xi_\mu^\gamma(x)\mu_{i0}^\gamma$$

for a priori known functions μ_{i0}^α, μ_{i0}^β and μ_{i0}^γ. Then all polynomials of order 4 $\xi_\mu^\alpha(x)$, $\xi_\mu^\beta(x)$ and $\xi_\mu^\gamma(x)$ can be determined uniquely to guarantee

$$\mu_{0i}(x_L) = \mu_{0i}^\alpha\,, \qquad \mu_{0i}(x_R) = \mu_{0i}^\gamma\,, \qquad \mu_{0i}(x_C) = \mu_{0i}^\beta\,, \qquad \mu'_{0i}(x_L) = \mu'_{0i}(x_R) = 0\,.$$

Moreover, if $\overline{\varphi}_i = \varphi_i(c)$ are set for fixed concentrations $c = (c_1, c_2, c_3)$, it is possible to write

$$\overline{\varphi}_i(x) = \xi_\varphi^\alpha(x)\overline{\varphi}_i^\alpha + \xi_\varphi^\gamma(x)\overline{\varphi}_i^\gamma$$

where no better information for the setting of polynomials of order 4 $\xi_\varphi^\alpha(x)$ and $\xi_\varphi^\gamma(x)$ is available than

$$\overline{\varphi}_i(x_L) = \overline{\varphi}_i^\alpha\,, \qquad \overline{\varphi}_i(x_R) = \overline{\varphi}_i^\gamma\,, \qquad \overline{\varphi}_i(x_C) = 0\,, \qquad \overline{\varphi}'_i(x_L) = \overline{\varphi}'_i(x_R) = 0$$

with $\overline{\varphi}_i^\alpha$ and $\overline{\varphi}_i^\gamma$ known from (rather complicated) experiments, arranged with respect to micromechanical arguments. (However, it is expected that these terms will not be dominant in the whole process of phase transformation, and therefore are negligible in the first rough approximation.)

Let us suppose that initial values of $c = (c_1, c_2, c_3)$ (such that $c_1 + c_2 + c_3 = 1$) are given; we shall denote them by $c^\times = (c_1^\times, c_2^\times, c_3^\times)$. Every diffusive flux, driven by concentration change, must satisfy the condition of mass conservation on Ω

$$\dot{c}_i + j'_i = 0\,.$$

On Ω also the Gibbs - Duhem condition $c_i\dot{\mu}_i = 0$ is valid.

The basic idea for the formulation of the evolution equations, following [4], p. 1374, and [5], p. 961, is the the evaluation of the total Gibbs energy of the system

$$G = \int_\Omega c_i\mu_i \,\mathrm{d}x$$

and its time derivative $\dot{G} = \dot{G}^\alpha + \dot{G}^\gamma + \dot{G}^I$ where

$$\begin{aligned}
\dot{G}^\alpha &= \int_0^{x_L} (\partial c_i/\partial t)\mu_i \,\mathrm{d}x + \dot{x}_L c_i(x_L)\mu_i(x_L) = -\int_0^{x_L} j'_i\mu_i \,\mathrm{d}x + v c_i(x_L)\mu_i(x_L)\,,\\
\dot{G}^\gamma &= \int_{x_R}^{H} (\partial c_i/\partial t)\mu_i \,\mathrm{d}x - \dot{x}_R c_i(x_R)\mu_i(x_R) = -\int_{x_R}^{H} j'_i\mu_i \,\mathrm{d}x - v c_i(x_R)\mu_i(x_R)\,,\\
\dot{G}^I &= \int_{x_L}^{x_R} (\partial c_i/\partial t)\mu_i \,\mathrm{d}x = -\int_{x_L}^{x_R} j'_i\mu_i \,\mathrm{d}x + v\int_{x_L}^{x_R} c_i\mu'_i \,\mathrm{d}x +\\
&\qquad v\,[c_i(x_R)\mu_i(x_R) - c_i(x_L)\mu_i(x_L)]
\end{aligned}$$

and of the rate of the total Gibbs energy dissipation due to bulk diffusion and interface migration

$$Q = \frac{1}{2}\int_\Omega (j_i^2/A_i) \,\mathrm{d}x + \frac{1}{2}\int_I (v^2/M) \,\mathrm{d}x + \int_\Omega \delta_{ii} j_i \lambda \,\mathrm{d}x\,.$$

The stationary point of the functional $\dot{G}+Q$ corresponds to zero values of all variational derivatives

$$\mathcal{D}(\dot{G}+Q)(\widetilde{j}_1,\widetilde{j}_2,\widetilde{j}_3) = \int_\Omega \widetilde{j}_i \mu_i' \,\mathrm{d}x + \int_\Omega (j_i \widetilde{j}_i / A_i)\,\mathrm{d}x = 0\,,$$

$$\mathcal{D}(\dot{G}+Q)(\widetilde{v}) = -\widetilde{v}\int_I c_i \mu_i' \,\mathrm{d}x + \widetilde{v}v/M = 0\,, \qquad \mathcal{D}Q(\widetilde{\lambda}) = \delta_{ii} j_i \widetilde{\lambda} = 0$$

for any admissible diffusional fluxes $\widetilde{j}_1,\widetilde{j}_2,\widetilde{j}_3$, an interface migration rate $\widetilde{v}$ and a Lagrange multiplier $\widetilde{\lambda}$.

One simple consequence of the second condition is the direct expression for calculation of interface migration rate

$$v = M\int_I c_i \mu_i' \,\mathrm{d}x\,.$$

The differential equations for concentrations on Ω can be derived from the remaining stationary point conditions: we have

$$\mu_i' + j_i/A_{\underline{i}} + \lambda = 0\,, \qquad \delta_{ii} j_i = 0$$

which (using the elimination of λ by [7]) yields

$$j_i = -A_{\underline{i}}A_k(\mu_i' - \mu_k')/(\delta_{ll}A_l) = -A_{\underline{i}}\left(\mu_i' - A_k\mu_k'/(\delta_{ll}A_l)\right)\,.$$

The integral version of the resulting differential equations, suggested in [7], is

$$\int_\Omega (\partial c_i/\partial t)\phi\,\mathrm{d}x + \int_\Omega A_{\underline{i}}A_k(\mu_i' - \mu_k')/(\delta_{ll}A_l)\phi'\,\mathrm{d}x = 0$$

for some virtual functions ϕ; after rather long calculations this can be converted into the form

$$\int_\Omega (\partial c_i/\partial t)\phi\,\mathrm{d}x + \int_\Omega B_{ik}(c)c_k'\phi'\,\mathrm{d}x = 0\,.$$

Nevertheless, $B_{ik}(c)$ are strongly nonlinear functions generated by μ_1, μ_2 and μ_3; this limits all applications of standard variational methods as FEM, FVM, etc. In the literature usually very simplified versions of such equations can be found. The analysis of the two-component system ($c_3 = 0$) is most frequent: since $c_2 = 1 - c_1$ evidently, only one evolution equation is substantial. For example, in [3] for a system of such type (using the theory of Hölder spaces and analytic semigroups in parabolic problems) both the existence and the uniqueness of smooth solutions for a fully nonlinear coupled system of PDEs has been proved. The proper three-component system (without deeper mathematical analysis) has been studied in [4]; unfortunately, its assumption of very thin interface ($x_L \to x_R$) cannot be removed and, moreover, standard differential equations are replaced by "ad hoc" constructed difference schemes, whose FDM convergence properties are not transparent.

3. Steady-state analysis. Most experiments with $\alpha \to \gamma$ transformations verify the hypothesis that (after some time) the process obtains steady-state properties – the quantities v and c become constant in time. The diffusional fluxes j_i are then able to be related to the concentrations c_i as

$$j_i = v(c_i - c_i^{\times})$$

where $c_i^\times$ are the concentrations in the phase γ far from the interface; the integral expression for the evaluation of v stays unchanged. Especially in the phase α no concentration profiles exist – the chemical composition is given by $c_i^\times$.

Let us try to construct an effective numerical algorithm for this case. We must respect that all diffusion coefficients $D_i(x)$ change their values on I very rapidly. Eliminating all explicit diffusional fluxes, we have now

$$A_{\underline{i}} A_k(\mu_i' - \mu_k')/(\delta_{ll} A_l) + v(c_i - c_i^\times) = 0\,.$$

To avoid long mathematical expressions, let us introduce several additional functions $\eta(c) = \zeta_l c_l$, $\widehat{\mu}_{0i}(x) = \mu_{0i}'/(RT)$ and $\sigma(c) = \widehat{\mu}_{0k}\zeta_k c_k$. Using the decomposition of μ_i (and dividing this equation by $D\zeta_i$), we obtain

$$c_i' - (c_i/\eta)\zeta_k c_k' + c_i\widehat{\mu}_{0k} - (c_i/\eta)\sigma + c_{\underline{i}}\varphi_{i,l}(c)c_l' - (c_i/\eta)c_k\zeta_k\varphi_{k,l}(c)c_l' + \\ vc_i/(D\zeta_i) = vc_i^\times/(D\zeta_i)$$

where $\varphi_{i,l}(c)$ means $\partial\varphi_i/\partial c_l$, etc. Clearly it is helpful to introduce one more notation

$$\widehat{\varphi}_{ik}(c) = c_i\varphi_{i,k}(c) - (c_i/\eta)c_l\zeta_l\varphi_{l,k}(c)\,;$$

this leads to a formally simple system of 3 ODEs with 3 unknowns

$$(\delta_{ik} - (c_i/\zeta_k)\eta + \widehat{\varphi}_{ik})\,c_k' + (\widehat{\mu}_{0i} - \sigma/\eta + v/(D\zeta_i))\,c_{\underline{i}} = vc_{\underline{i}}^\times/(D\zeta_i)\,.$$

Evidently, $c_1 + c_2 + c_3 = 1$, and thus $c_3' = -c_1' - c_2'$. This enables us to remove the last (third) equation and to express c_3 (including its derivative) in first two equations by means of remaining concentrations. Standard algebraic manipulations then yield

$$(\mathcal{I} + \mathcal{M})\bar{c}' + \mathcal{K}\bar{c} = \mathcal{F}$$

where $\bar{c} = (c_1, c_2)$ (later also $\bar{c}^\times = (c_1^\times, c_2^\times)$ will be useful), $\mathcal{M}$ is the square matrix of order 2 compound from elements ($i, k \in \{1, 2\}$)

$$\mathcal{M}_{ik} = -c_i\,(\zeta_i - \zeta_3)\,/\eta + \widehat{\varphi}_{ik} - \widehat{\varphi}_{i3}\,,$$

$\mathcal{K}$ is the diagonal square matrix of the same order compound from elements ($i \in \{1, 2\}$)

$$\mathcal{K}_i = \widehat{\mu}_{0i} - \sigma/\eta + v/(D\zeta_i)$$

and $\mathcal{F}$ is the vector consisting of 2 elements ($i \in \{1, 2\}$ again)

$$\mathcal{F}_i = vc_i^\times/(D\zeta_i)\,.$$

The exact solution of such system is (even in case of constant μ_{0i} and zero ϕ_i) not available; therefore some robust numerical scheme has to be applied. In [7] the formal transformation $z_i = \zeta_{\underline{i}} c_i$ has been done and the whole system has been reformulated in new variables z_i. This can simplify the system for (nearly) piecewice constant factors ζ_i. However, in case of rapid changes of ζ_i the original formulation with unknown concentrations c_i seems to be better for the following numerical analysis: in practice we can expect $\varepsilon/2 < c_i < 1 - \varepsilon$ with $\varepsilon \approx 10^{-3}$, thus e.g. $(\max_{x\in I}\max(c_1, c_2, c_3))/(\min_{x\in I}\min(c_1, c_2, c_3))$ will be probably much lower than $(\max_{x\in I}\max(z_1, z_2, z_3))/(\min_{x\in I}\min(z_1, z_2, z_3))$.

For example, the Crank-Nicholson scheme on I gives

$$(\mathcal{I}+\mathcal{M}^s+\frac{\Delta}{2}\mathcal{K}^s)\bar{c}^s=(\mathcal{I}+\mathcal{M}^{s-1}-\frac{\Delta}{2}\mathcal{K}^{s-1})\bar{c}^{s-1}+\mathcal{F}^s\,;$$

here Δ means a calculation step and ψ^s is briefly used instead od $\psi(s\Delta)$ for any function $\psi(x)$ everywhere on Ω and $s \in \{1,\dots m\}$, $m=h/\Delta$ (therefore $c'(sh)\approx(c^s-c^{s-1})/\Delta$). At the start of all calculations both matrices $\mathcal{M}^s$ and $\mathcal{K}^s$ are set using the assumption that $c_i=c_i^{\times}$ (no better information is available); this starts an iterative procedure of evaluation of $\bar{c}^1,\bar{c}^2,\dots,\bar{c}^m$ and also v, correction of $\mathcal{M}^1,\dots,\mathcal{M}^m$, of $\mathcal{K}^1,\dots,\mathcal{K}^m$ and of $\mathcal{F}^1,\dots,\mathcal{F}^m$, etc. Outside I (where $H\gg h$) the real distributions of concentrations are typically similar to (but not exactly identical with) exponential curves: the first two additive terms in $\mathcal{K}_i$ are equal to zero, the right-hand side of the whole system of ODEs is constant, the (non-constant) matrix $\mathcal{M}$ is not far from diagonal (neglecting all terms of type $\widehat{\varphi}_{ik}$), thus the eigenvalue analysis for $-(\mathcal{I}+\mathcal{M}^s)^{-1}\mathcal{K}^s$ can be useful to improve approximate solutions from the Crank-Nicholson scheme.

4. Numerical results and discussion. All numerical calculations make use of the original software code, runable in each standard MATLAB environment (with no special requirements to additional toolboxes of FEMLAB compatibility). Only the automatic code generator of algebraic expressions for μ_i evaluation (not described in details here) needs MAPLE-supported symbolic differentiation.

As a typical example, let us consider 3 chemical potentials defined by

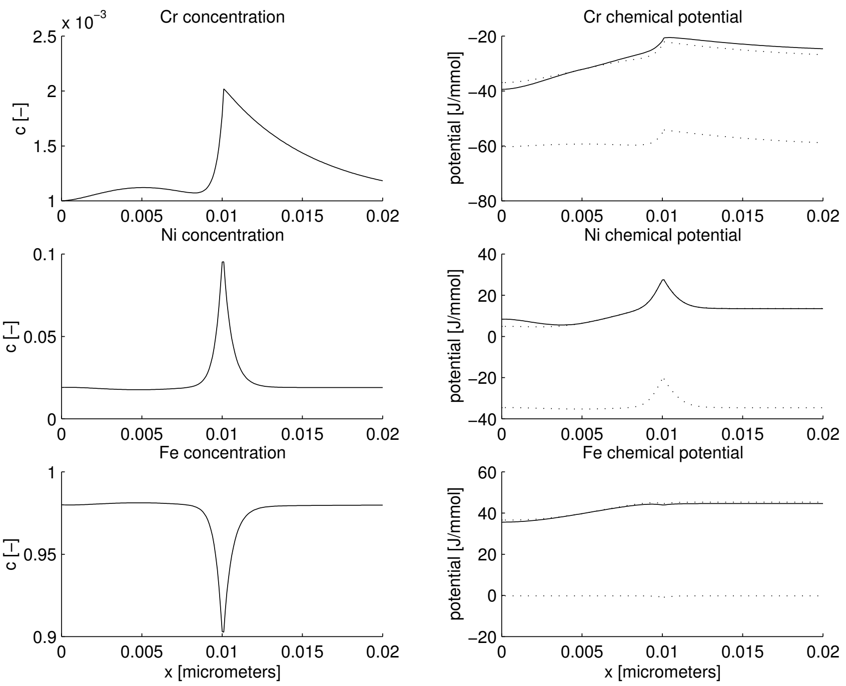
$$\begin{array}{lcllcllcl}
\mu_{01}^{\alpha} &=& 23353\ \mathrm{J/mol}\,, & \mu_{01}^{\beta} &=& 39437\ \mathrm{J/mol}\,, & \mu_{01}^{\gamma} &=& 36765\ \mathrm{J/mol}\,,\\
\mu_{02}^{\alpha} &=& 27186\ \mathrm{J/mol}\,, & \mu_{02}^{\beta} &=& 41624\ \mathrm{J/mol}\,, & \mu_{02}^{\gamma} &=& 39885\ \mathrm{J/mol}\,,\\
\mu_{03}^{\alpha} &=& 32083\ \mathrm{J/mol}\,, & \mu_{03}^{\beta} &=& 48167\ \mathrm{J/mol}\,, & \mu_{03}^{\gamma} &=& 45495\ \mathrm{J/mol}\,,
\end{array}$$

the interface thickness $h=H/2=10^{-8}$ m (the value of H must be supplied for the postprocessing) and the mobility coefficient $M=4.10^{-14}\ \mathrm{J\,s/m^4}$. The values of diffusive coefficients can be transformed from those applied in [5], p. 965:

$$\begin{array}{lcllcllcl}
D_3^{\alpha} &=& 10^{-14}\ \mathrm{m^2/s}\,, & D_3^{\beta} &=& 10^{-16}\ \mathrm{m^2/s}\,, & D_3^{\gamma} &=& 4.10^{-19}\ \mathrm{m^2/s}\,,\\
D_1^{\alpha} &=& 2D_3^{\alpha}\,, & D_1^{\beta} &=& 2D_3^{\beta}\,, & D_1^{\gamma} &=& 5D_3^{\gamma}\,,\\
D_2^{\alpha} &=& .3D_3^{\alpha}\,, & D_2^{\beta} &=& .3D_3^{\beta}\,, & D_2^{\gamma} &=& .5D_3^{\gamma}\,.
\end{array}$$

All functions φ_i^{α} and φ_i^{γ} are available for our Fe-Cr-Ni system as the research outputs from the Montainuniverisität Leoben (thanks to the collaborations with the joint authors of [6]). Unfortunately, their original calculation formulae are very long (containing more then 1500 FORTRAN program lines, much more complicated than those presented in the illustrative example of [7]) and include a lot of additive terms of power-law types $(\dots)\,c_i^r$ and $(\dots)\,c_i^r\ln c_i$ with $r\in\{0,1,\dots,25\}$. Therefore it was necessary to prepare a special MATLAB-based software to analyse these formulae, to decompose them into logical parts and to suggest some algorithms for the (not very expensive) evaluation of φ_i and (using the symbolic differentiation) of $\varphi_{i,k}$. As we have announced yet, we shall start from $c_1^{\times}=0.001$ and $c_2^{\times}=0.019$.

For such data the final distributions of concentrations of Cr, Ni and Fe have been obtained after 3 iterative steps; the results are evident from Fig. 1 where these distributions in the left column are completed by the distributions of corresponding chemical potentials μ_i: the full line shows always the final value, the upper dashed


Cr concentration

Cr chemical potential

Ni concentration

Ni chemical potential

Fe concentration

Fe chemical potential

Fig. 1. *Original settings of material characteristics*

line shows the approximate final value without any correction based on φ_i functions (from the above mentioned complicated formulae) and the lower dashed line shoes the value of $RT \ln c_i$ only. Fig. 2 and Fig. 3 demonstrate that relatively small changes of material characteristics cause very different results: those on Fig. 2 were received for $M = 4.10^{-15}$ J s/m^4 (instead of original $M = 4.10^{-14}$ J s/m^4), those on Fig. 3 for $D_3^{\gamma} = 2.10^{-18}$ m^2/s (instead of original $D_3^{\gamma} = 4.10^{-19}$ m^2/s).

Some more results of numerical simulations have been published in [6]. Both M and $D^{\beta}_{\underline{i}}/D^{\alpha}_{i}$ have been supposed as free parameters to study the changes in the behavior of all concentration profiles. Alternatively, to provoke a significant solute segregation, other chemical potentials than those from our example have been tested, too. Several figures and graphs presented in [6] (together with other sequences of results of computations, not published yet) show how the concentration profiles are influences by the above mentioned settings. (Let us remind the fact that most material characteristics for the $\alpha \rightarrow \gamma$ phase transformation are far from exact – various authors rely on various "correct values".) In the case that no solute drag effect is supposed and a finite interface mobility is assumed, the sharp interface model [5] predicts the same jumps of chemical potentials for all substitutional components across the interface. These conditions can be modified dramatically if the solute segregation and drag effects are included into the model. The jumps of chemical potentials are then not the same for all components and depend on both M and $D^{\beta}_{\underline{i}}/D^{\alpha}_{i}$.

We can conclude: to reach a higher level of understanding of Fe-rich Fe-Cr-Ni phase transformation, it seems to be necessary at least: i) to do more precious analysis of sensitivity of all concentration profiles on prescribed material characteristics (including complicated "nonlinear corrections" φ_i of chemical potentials and their

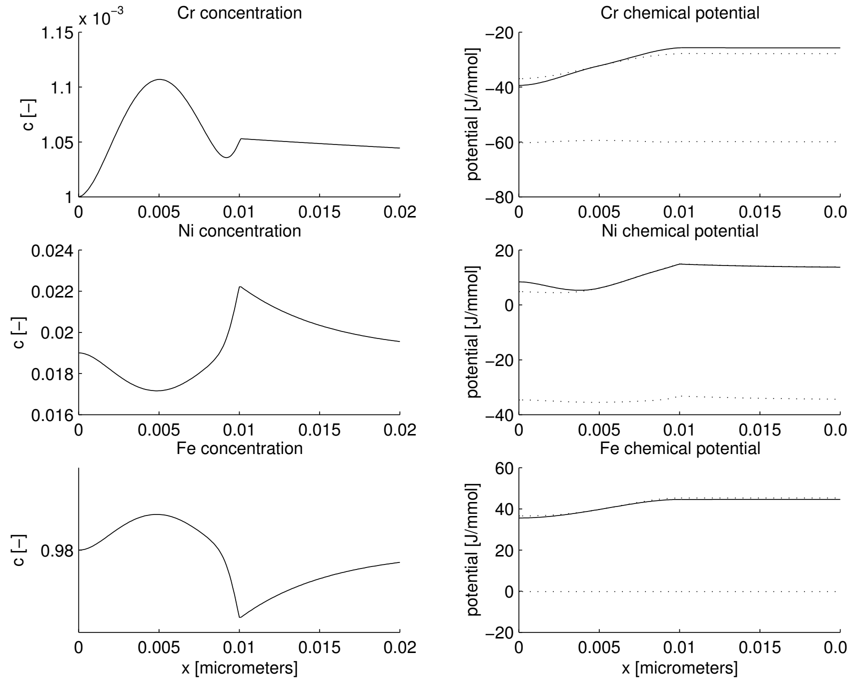


FIG. 2. *Modified interface mobility*

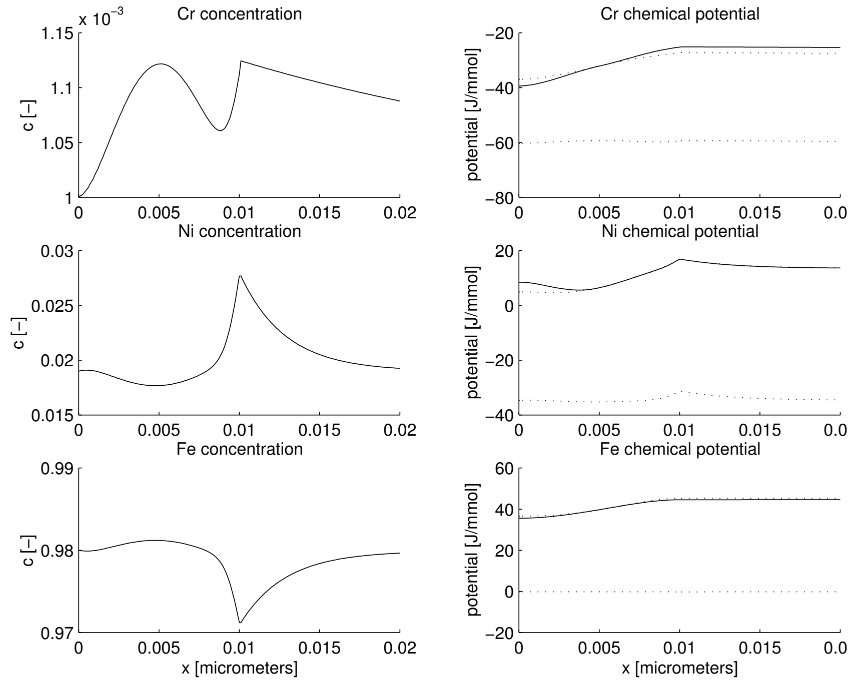


FIG. 3. *Modified diffusive coefficients in the phase* γ

physical background), ii) to prepare a special FEM software for the analysis of the original evolution (not only of the simplified steady-state) problem.

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