TWO-SCALE CONVERGENCE IN HEAT TRANSFER

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Abstract

The reliable analysis of heat transfer in real materials cannot avoid the information about their microstructure. The global computational modelling, covering both the microstructural material properties and the macrostructural behaviour of the whole specimen or even of the complete construction, is usually very expensive or even impossible in practice. This is the principal motivation for the development of the mathematical theory of homogenization, which describes the replacement of a real composite material by a fictious homogeneous one. The approach based on the notion of the two-scale convergence, covering the gap between the weak and the strong convergence in the case of the periodic or quasi-periodic material structure, seems to be useful and physically transparent not only for the pure heat transfer, both for the steady-state and the time-dependent ones, but also for its coupling with other important physical processes. However, most such multiphysical problems contain still a lot of open questions and some microstructural formulations seem not to be able to be homogenized easily.

Key words: Heat transfer, homogenization techniques, two-scale convergence.

1. Mathematical modelling of heat transfer

Advanced materials used in engineering have typically a complicated microstructure, whose simple and intuitive macroscopic representation is not available. On the other side, the distributions of macroscopic quantities, as temperature, strains and stresses, moisture content, concentrations of components or contaminants, etc., are required as final outputs of technical calculations. The simultaneous numerical computations covering the scales from micro- or nanometers (in the case of the microstructural analysis) to meters (for the material specimen or even for the complete construction, typically for some building object in civil engineering) are usually not available: they are very expensive even for the relatively simple model problems and impossible for the realistic computations required by engineering and technological applications. This is the principal motivation for the development of physically transparent computational and numerical techniques of scale bridging, known as the mathematical homogenization (despite the fact that not it all cases the limit description corresponds to quite physically homogeneous material properties).

The history of intensive research in the mathematical homogenization is relatively short, being connected with the technological progress both in the development of advanced materials and in the computer hardware and software. Most authors start with the citation of [3] as the pioneering work in homogenization motivated by engineering problems; however, in the particular cases certain analogous approaches can be found in some old studies from the beginning of the 20th century, namely in [39] for the one-dimensional heat propagation through a layered medium. In this paper, especially at the beginning, we shall pay (for simplicity) attention to the pure heat transfer in a physically isotropic domain Ω located in the three-dimensional Euclidean space R^3 with a (sufficiently smooth, e.g. Lipschitz) boundary $\partial\Omega$; thus the Cartesian coordinate system $x = (x_1, x_2, x_3)$ is available, the classical differential operators (∇, div, $\cdot$ for scalar products, …) can be used and the analysis of the existence and

uniqueness of solution, of the convergence of sequences of approximate solutions, etc., can refer to the standard results from the theory of function spaces by [19], namely of the Lebesgue and Sobolev ones, discussed in great details in [23]; the commonly used notation of function spaces will be applied here without further explanation.

We shall consider the boundary $\partial\Omega$ divided into two parts, Γ and Γ_*, where $\partial\Omega = \Gamma \cup \Gamma_*$. The heat transfer is driven by the external heat flow $q(x)$ on Γ and by the internal heat source $r(x)$ in Ω. We are seeking for the distribution of temperature $T(x)$, conditioned by the heat conduction factor $\lambda(x)$ on Ω, with respect to the prescribed temperature $T_*(x)$ on Γ_*, extensible formally to Ω. The differential formulation of the problem can be then written as

$$-\mathrm{div}(\lambda\nabla(\tau + T_*)) = r \tag{1}$$

on Ω and

$$\nabla\lambda \cdot \nu = q \tag{2}$$

on $\partial\Omega$, supplied with the unit normal vector ν; the new variable $\tau = T - T_*$ is introduced to force $\tau = 0$ on Γ_*. Let us remark that in general (1) and (2) (for a non-smooth τ) should be understood only in a distributive sense (not very transparent for the physicists and engineers); nevertheless, this can be removed by the integral formulation, coming from the Green-Ostrogradskiĭ theorem: we have to find such $\tau \in V$ that

$$(\nabla v, \lambda\nabla\tau) = (v, r) + < v, q > -(\nabla v, \lambda\nabla T_*) \tag{3}$$

holds for all $v \in V$; assuming $r \in L^2(\Omega)$, $q \in L^2(\Gamma)$, $T_* \in W^{1,2}(\Omega)$ and some positive bounded λ on Ω and applying the notation of scalar products

$$(\varphi, \psi) = \int_\Omega \varphi(x)\psi(x)\ \mathrm{d}x$$

for all $\varphi, \psi \in L^2(\Omega)$ and

$$(\varphi, \psi) = \int_\Gamma \varphi(x)\psi(x)\ \mathrm{d}\sigma(x)$$

for all $\varphi, \psi \in L^2(\Gamma)$ (σ means the Hausdorff surface measure), we have aa appropriate space of test functions

$$V = \{v \in W^{1,2}(\Omega) : v_1 = v_2 = v_3 = 0 \text{ on } \Gamma_*\}.$$

The solution of (3) is relatively easy and can be performed numerically by probably every software package for the analysis of problems of building physics, continuum mechanics and related fields. The main difficulty is that we do not know how to set λ at the macroscopic scale to incorporate the information from the microscopic one. The naive averaging gives evidently bad results: e.g. the well-known result

$$\frac{2}{\lambda} = \frac{1}{\lambda_1} + \frac{1}{\lambda_2},$$

valid, following [39], for a specimen of the thickness h consisting of a large number n of parallel layers of the same thickness $\varepsilon = h/(2n)$ where the odd and even ones have their heat conduction factors $\lambda_1, \lambda_2, \ldots, \lambda_1, \lambda_2$ with $n \to \infty$ (alternatively: $\varepsilon \to 0$) and the heat transfer is

considered only in the direction perpendicular to such system of layers, is quite different from the arithmetical average

$$\lambda = \frac{\lambda_1 + \lambda_2}{2};$$

both results coincide just for $\lambda_1 = \lambda_2$, i.e. for the a priori ideal homogeneous medium.

The assumption on the steady-state heat transfer may be not acceptable in a lot of cases of practical importance. Namely in the analysis of the heat transfer in building the setting of λ reflects only the effect of thermal insulation, not that of (time-dependent) thermal accumulation. Thus (1) has to be extended to the form

$$\kappa(\dot{\tau} + \dot{T}_*) - \mathrm{d\,v}(\lambda \nabla(\tau + T_*)) = r \tag{4}$$

with the dot convention for the partial derivative with respect to the time t increasing from zero to some final time t_*, where at least q, r and consequently also T are allowed to be functions of the time variable t; κ here is introduced as $\kappa(x) = c(x)\rho(x)$ where $c(x)$ is the heat capacity and $\rho(x)$ the material density on Ω. Since (2) stays formally unchanged, (3) converts to

$$(v, \kappa\dot{\tau}) + (\nabla v, \lambda \nabla \tau) = (v, r) + < v, q > -(v, \kappa \dot{T}_*) - (\nabla v, \lambda \nabla T_*) \tag{5}$$

for all $v \in V$; for the time interval $I = [0, t_*]$ and the zero-valued τ in the initial time $t = 0$ we must consider $r \in L^2(I, L^2(\Omega))$, $q \in L^2(I, L^2(\Gamma))$, $T_* \in L^2(I, W^{1,2}(\Omega))$ and some bounded λ and c on Ω and try to find $\tau \in L^2(I, V)$ and consequently $T \in L^2(I, W^{1,2}(\Omega))$. The discussion concerning the identification of λ can be then repeated for κ (or separately for c and ρ), too.

2. Classical homogenization techniques

The first attempt to overcome the difficulty with the identification of some effective value of λ can be done in the following way: we can start from the correct fine ε-scaled configuration where τ^ε is nothing else τ from (3) (or alternatively (1) and (2)) with known λ^ε which refers just to exact λ (often considered as periodic or quasi-periodic on Ω in practice), thus

$$(\nabla v, \lambda^\varepsilon \nabla \tau^\varepsilon) = (v, r) + < v, q > -(\nabla v, \lambda^\varepsilon \nabla T_*)\ , \tag{6}$$

and the aim is to find such λ that the sequence $\lambda^\varepsilon \nabla \tau^\varepsilon$ from (6) converges weakly to $\lambda \nabla \tau$ from (3) in $L^2(\Omega)$. This type of convergence, known as H-convergence in the literature, has found wide acceptance in the composites modelling community, for its ability to incorporate and estimate effective material properties from a representative unit cell, as suggested in [3]. The classical works [4] and [30] are commonly cited to demonstrate that such H-limits λ of corresponding sequences λ^ε where $\varepsilon \to 0$ can be calculated explicitly for periodic systems, although their evaluation is much more complicated than in the one-dimensional case in the historical work [39]. However, in general the derivation of H-limits is not explicit and requires to solve additional non-trivial problems; all details (including the comparison of H-, G- and two-scale limits, the formal mathematical existence and convergence proofs and engineering applications) can be found in [7].

The complicated evaluation of H-limits has motivated the improvements of the concept of H-convergence; here we shall mention only two important directions. For the convergence of λ^ε in the corresponding space of linear operators (or the convergence of the Green operator) the literature (not only for the heat transfer, but in the more general context) refers to G-convergence (cf. [32] and [9])). The convergence of the triples $(\lambda^\varepsilon \nabla \tau^\varepsilon, \nabla \tau^\varepsilon, \tau^\varepsilon)$ is known as Γ-convergence (cf. [24], [10] and [8]). Nevertheless, in such classification the announced two-scale convergence could be interpreted as a specific case of H-convergence, taking usually in account some (quasi-)periodicity of the solution and working with certain rather strange limit functions; in the following text we shall demonstrate a greater significance of the two-scale analysis.

Let us remark that, namely in the last two decades, the above mentioned method have been generalized substantially to handle much more general problems than that formulated by (6) and (3); however, we shall not discuss such generalizations in details to preserve the simplicity and transparency of our notations. Only for the future reference we shall rewrite (5) to the slightly generalized version of (6),

$$(v, \kappa^\varepsilon \dot{\tau}^\varepsilon) + (\nabla v, \lambda^\varepsilon \nabla \tau^\varepsilon) = (v, r) + < v, q > -(v, \kappa^\varepsilon \dot{T}_*) - (\nabla v, \lambda^\varepsilon \nabla T_*) \tag{7}$$

where not only one sequence λ^ε, but a couple of sequences $(\lambda^\varepsilon, \kappa^\varepsilon)$ of material characteristics, coming from the fine scale, but tending to some effective (λ, κ) for (5), occurs.

3. Two-scale convergence analysis

The two-scale convergence was introduced originally in [26], but this pioneering work (whose form is not very reader-friendly) has not been accepted as an important tool in the homogenization theory immediately. Most authors, using the mathematical two-scale homogenization and the corresponding convergence results to the analysis of physical or technological problems, or even those trying to generalize the formal definition of a (strong or weak) two-scale limit, refer to the later rather extensive overview [1]; its notation will be therefore applied also in this paper. Some useful generalizations will be discussed later.

Let Y be the unit cube in R^3: $Y = [0,1) \times [0,1) \times [0,1)$. This cube should correspond to certain representative volume (small in practice) at the fine scale; thus it would be physically more convenient to take some cube of a realistic volume, but according to $\varepsilon \to 0$ the additional assumption $\mathrm{vol}\, Y = 1$ brings no loss of generality and simplifies most equations. The space of Lebesgue square integrable Y-periodic functions will be denoted by $L^2(Y_\#)$. Its elements are Y-periodic; its restriction to Ω belongs to $L^2(\Omega)$, although its norm is constructed over Y only.

Let us now introduce the two-scale convergence; ε will be a positive real constant (everywhere in this paper). Let S be certain space of admissible functions from $L^2(\Omega \times Y)$. A sequence u^ε is said to *two-scale converge* to a limit $u^0 \in L^2(\Omega \times Y)$ iff

$$\lim_{\varepsilon \to 0} \int_\Omega u^\varepsilon(x) \varphi(x, x/\varepsilon)\ \mathrm{d}x = \int_\Omega \int_Y u^0(x, y) \varphi(x, y)\ \mathrm{d}y\ \mathrm{d}x \tag{8}$$

for all $\varphi \in S$. The choice of S by various authors is different; for our purpose $S = C(\Omega, L^2(Y_\#))$ will be sufficient. Let us remark that the seemingly simplest setting

$S = L^2(\Omega \times Y)$ is not acceptable, unlike $S = L^2(\Omega, L^2(Y_\#))$ (for the detailed explanation see [13]).

An alternative definition can be rewritten from [2]: Let us consider the system of k-shifted and ε-scaled cells $Y_k^\varepsilon = \varepsilon(Y + k)$ for all triples of integers $k = (k_1, k_2, k_3)$; this system covers the whole space R^3, containing Ω. Let a^ε be a measure preserving mapping of $\Omega \times Y$ onto Ω defined by $a^\varepsilon = \varepsilon(y + k)$ for $x \in Y_k^\varepsilon$ if Y_k^ε is included in Ω (i.e. contained in inner cells) and as $a^\varepsilon = x$ for $x \in Y_k^\varepsilon \cap \Omega$ (i.e. contained in boundary cells). Let A^ε be a transform of $L^2(\Omega, L^2(Y_\#))$ into $L^2(\Omega \times Y)$ defined by

$$(A^\varepsilon v^\varepsilon)(x, y) = v^\varepsilon(a^\varepsilon(x, y))$$

for any sequence v^ε in $L^2(\Omega)$. A sequence u^ε is said to *weakly two-scale converge* to a limit $u^0 \in L^2(\Omega \times Y)$ iff $A^\varepsilon u^\varepsilon$ weakly converges to $L^2(\Omega \times Y)$. A sequence u^ε is said to *strongly two-scale converge* to a limit $u^0 \in L^2(\Omega \times Y)$ iff $A^\varepsilon u^\varepsilon$ strongly converges to $L^2(\Omega \times Y)$.

As verified in [25], the weak two-scale convergence can be identified with the two-scale convergence by (8). The strong two-scale convergence can be characterized as the (weak) two-scale convergence with the additional requirement

$$\lim_{\varepsilon \to 0} \left\| u^\varepsilon \right\|_{L^2(\Omega)} = \left\| u^0 \right\|_{L^2(\Omega \times Y)}.$$

The most useful lemmas working with the two-scale convergence with $\varepsilon \to 0$ are:

On the compactness: If u^ε is a bounded sequence in $L^2(\Omega)$ then, up to a subsequence, u^ε two-scale converges to some u^0 in $L^2(\Omega \times Y)$

On the function products: If u^ε is a strongly two-scale converging sequence to some $u^0 \in L^2(\Omega \times Y)$ and v^ε is a two-scale converging sequence to some $v^0 \in L^2(\Omega \times Y)$ then

$$\int_\Omega u^\varepsilon(x) v^\varepsilon(x)\, \mathrm{d}x = \int_\Omega \int_Y u^0(x, y) v^0(x, y)\, \mathrm{d}y\, \mathrm{d}x\ .$$

On the weak and strong convergence: If u^ε is a strongly converging sequence to some u in $L^2(\Omega)$ then also u^ε strongly two-scale converges to u^* in $L^2(\Omega \times Y)$ where $u^*(x, y) = u(x)$ for every $x \in \Omega$ and $y \in Y$ If at least u^ε is a two-scale converging sequence to some u^0 in $L^2(\Omega \times Y)$ then u^ε weakly converges to u in $L^2(\Omega)$ where

$$u(x) = \int_Y u_0(x, y)\, \mathrm{d}y$$

for each $x \in \Omega$.

On the gradients: If u^ε is a bounded sequence in $L^2(\Omega)$ and moreover ∇u^ε is bounded in $L^2(\Omega, R^3)$ then, up to subsequences, u^ε has certain two-scale limit in u^* in $L^2(\Omega \times Y)$, whose restriction u to $L^2(\Omega \times Y)$ comes from the preceding lemma, and also ∇u^ε has a (vector-valued) two-scale limit $\nabla u^* + \nabla_y u^1$ where the gradient ∇_y is computed with respect to the second variable $y \in Y$ and u^1 is certain element of $L^2(\Omega, W^{1,2}_\#(Y))$.

The careful application of these lemmas enables us to understand (3) as the two-scale limit version of (6) and verify the existence of an effective λ on Ω for a sequence of quasi-

periodic heat conduction factors λ^ε defined by

$$\lambda^\varepsilon(x) = \lambda(x, x/\varepsilon)$$

for all $x \in \Omega$. Moreover, the strong convergence in $L^2(\Omega \times Y)$ can be helpful, too (especially later in the numerical analysis). However, the guaranteed solution of (3) τ contains its oscillatory part τ^1 (cf. the lemma on the gradients), periodic on Y. The meaning of τ^1 is often explained using the formal asymptotic expansion (see [1])

$$\tau^\varepsilon(x)(x) = \tau^0(x, x/\varepsilon) + \varepsilon\tau^1(x, x/\varepsilon) + \varepsilon^2\tau^2(x, x/\varepsilon) + \dots,$$

taking only first two right-hand-side additive terms with τ^0 and τ^1 into account. This leads naturally to the suggestion to include more terms into consideration; such approach, known as reiterated homogenization, has its good support inside the two-scale analysis.

4. Useful generalizations

The generalization of the above introduced two-scale analysis is available in several directions. Some small improvements are clear and simple: e.g. the isotropy assumption can be easily removed, replacing the scalar factor λ by certain symmetrical matrix from $R^{3\times3}$, q can contain a τ-variable term, incorporating the heat convection from the environment (or from the adjacent layer), etc. It is also possible to admit that λ is a function of T or even to replace $\lambda\nabla\tau$ totally by some function

$$l(x, \tau(x), \nabla\tau(x)),$$

respecting some additional requirements, e.g. of the Carathéodory type, and replace also the spaces $L^2(\Omega)$, $L^2(\Gamma)$, $W^{1,2}(\Omega)$, etc., by the slightly generalized spaces $L^p(\Omega)$, $L^p(\Gamma)$, $W^{1,p}(\Omega)$, etc., with $1 < p < \infty$. More serious complications can be connected with the perforated domains (let us remind that most building materials have a non-negligible pore space) and with the materials containing stiffening thin plates or long fibers located in the matrix: the analysis of such problems requires to substitute the standard Lebesgue and Sobolev spaces by some more general spaces working with the generalized Borel, Young, etc. measures; for more information see [13], [5] and [20]. However, the strong and relatively simple results like [6] cannot be then expected. This is caused by the loss of (quasi-)linearity of the problem and by the absence of the standard compactness arguments from the theory of Hilbert (or at least reflexive Banach) spaces; for more details and references see [37].

Another very useful generalization is the passage from the steady-state heat transfer to the analysis of the time-variable redistribution of temperature, from the mathematical point of view from an elliptic to a parabolic problem. The theoretical two-scale convergence results are available from [16] (even admitting the time-scaled changes of material characteristics); this enables us the passage from (6) and (3) to (7) and (5). The construction of the solution of a parabolic problem from a sequence of approximate solutions of corresponding elliptic problems, based on the method of discretization time and applying the properties of sequences of Rothe, is demonstrated in [35].

Unfortunately, also the periodicity assumption may be far from realistic ones; that the regular location of particles in the material can predict quite other outputs than their stochastic distributions. This is an important motivation for the development of the two-scale analysis without the deterministic periodicity. We have seen the incorrect results of the naive avaraging just in

the very simple case of one-dimensional heat propagation; the more complicated anisotropic configurations then need the support of advanced correlation analysis (see [18]). The approach of [17] and [31] tries to solve the sketched problem in the compatible way with the standard notations in the Lebesgue and Sobolev spaces, replacing the Lebesgue, Hausdorff, etc. measures by the probabilistic ones, applying the arguments from the theory of stochastic processes. Another method is presented in [27]: using the basic concept, called homogenization structure, and the deep results from the theory of Banach algebras, the so-called Σ-convergence promises to handle all known non-periodic formulations, including the probabilistic one (via the Radon measures and the Gelfand representations of special algebras). This concept evidently involves the two-scale convergence as a very special case; however, its application to most non-periodic engineering problems is not quite transparent and the whole text expects the very experienced reader, familiar with the methods and results from various branches of pure and applied mathematics; this may be the reason why e.g. the latest monograph on multiscale methods [28] ignores these results at all.

Moreover, the coupling of the heat transfer with other physical processes brings still new problems. Especially the complex analysis of heat, air and moisture propagation (the so-called HAM modelling, possibly accompanied with some contaminant) in buildings, based on the classical thermodynamical principles, namely on the conservation of mass, inertia and energy, leads, even in the case of a priori known macroscopic material characteristics, to some mathematical problems, whose solvability is not clear; for the more proper overview see [38]. The same is true e.g. for the hygro-thermo-mechanical modelling of the early-age concrete, conditioning all later mechanical properties and the durability of the whole structure, discussed in [14]. Typically the treatment of such complicated problems uses various semi-empirical ad hoc simplifications beyond the scope of this paper.

5. Numerical treatment

The number of papers presenting the computational algorithms and the results from the software applications performing the modelling and simulation of engineering problems is much higher than the proper mathematical and physical studies, referenced in this paper. The very frequent engineering approach consists of some experimental computations at various scales, applying rather artificial boundary conditions to commercial software packages, composed by the classical least squares method. Their (more or less strange) result generate good arguments for the minority of critical opinions like [12]: “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”.

Omitting the ad hoc computations with no or weak theoretical support, we must notice some studies of the two- or more-scale techniques, namely in the finite element method (but also e.g. in the finite volume or finite difference methods or their various combinations). Some of them do not apply any proper homogenization, being concentrated to the analysis of the (possibly parallelized) computations on two or more not necessarily nested grids. A very useful iterative algorithm, based on the improved Schwarz-Cauchy inequality, has been suggested in [15]; as shown in [36], it can be adopted also to the finite element analysis of linear problems incorporating the two-scale approach, i.e. to the formulations like (6) and (3). The four crucial steps of this algorithm (in the very simplified version) after the setting of the first estimate τ_*^0 of τ are:

1. find such $\tau^\varepsilon \in V^\varepsilon$ that

$$(\nabla v^{\varepsilon}, \lambda^{\varepsilon} \nabla \tau^{\varepsilon}) = (v^{\varepsilon}, f) + < v^{\varepsilon}, q > -(\nabla v^{\varepsilon}, \lambda^{\varepsilon} \nabla T_{*}) - (\nabla v^{\varepsilon}, \kappa^{\varepsilon}, \nabla \tau_{*}^{0})$$

for all $v^{\varepsilon} \in V^{\varepsilon}$,

2. set $\tau_{*}^{1/2} = \tau_{*}^{0} + \omega \tau^{\varepsilon}$,

3. find such $\tau^{h} \in V^{h}$ that

$$(\nabla v^{h}, \lambda \nabla \tau^{h}) = (v^{h}, f) + < v^{h}, q > -(\nabla v^{h}, \kappa \nabla T_{*}) - (\nabla v^{h}, \lambda \nabla \tau_{*}^{1/2})$$

for all $v^{h} \in V^{h}$,

4. set $\tau_{*}^{1} = \tau_{*}^{1/2} + \omega \tau^{h}$,

etc. (obtaining $\tau_{*}^{3/2}, \tau_{*}^{2}, \ldots$, until the error is significant); here $\omega \in (0,2)$ is an appropriate relaxation parameter, V^{ε} and V^{h} are the finite-dimensional subspaces of V corresponding to the fine scale and to the rough scale, respectively (ε and h can be identified with the norm of decomposition of Ω to finite elements, ε being much lesser than h, but the convergence analysis works with simultaneous $\varepsilon \to 0$ and $h \to 0$ theoretically), and the a priori knowledge of the effective value λ is assumed for simplicity. If the last statement is not true then the construction of the approximate solution of certain non-trivial additional problem should to be incorporated into the algorithm; for more details see [21] and [22].

The convergence analysis of the algorithms of the above sketched type enables us, at least for the linear problems, to derive convergence results comparable with those known from the classical finite element analysis. Some results beyond the linear formulations, both for the steady-state and for the time-dependent formulations, can be found in [11]; nevertheless, the formal verification of the existence of two-scale limits is available for a much larger class of problems than the convergence for such fully discretized schemes.

6. Still open problems

We have mentioned several complex problems, whose theoretical analysis seems to contain still more open questions than complete answers. Other typical problems of this type are those containing some non-local phenomena, occurring often in the simulation of the initiation and development of fracture, of the high-temperature phase transformation, etc. Even seemingly simple one-dimensional problems can lead to the results where any reasonable two-scale analysis is not available.

As an example we shall present the modelling of diffusive and massive phase transformation, whose physical fundamentals are introduced in [33]. The evolution of q substitutional and r interstitial, totally $q-1+r$, molar fractions c in one dimension 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 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 between $x^{L}(t)$ and $x^{R}(t)$. One missing molar fraction comes from the additional condition $c_1 + \ldots c_q = 1$. The resulting system of equations, starting from some a priori known initial values of c, reads

$$Bc' + (K + vN)c - N\frac{C}{\tau} = vNc^{\Diamond} - N\Omega j^{\Diamond} - N\frac{C^{\times}}{\tau} \tag{9}$$

where all variables are evaluated in time t, except $C^{\times} = C(t-\tau)$, τ denotes the time interval, referring (for simplicity here) to the implicit Euler method (the system of differential equations can be derived from such difference ones using the limit passage $\tau \to 0$); 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

$$C(x,t) = \int_0^x c(\xi,t)\mathrm{d}\xi \,, \tag{10}$$

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

$$v = \frac{\Omega}{M} \sum_{i=1}^{q+r} \int_0^h c_i \mu_i' \ \mathrm{d}x \tag{11}$$

for the prescribed chemical potentials μ_i as complicated functions of c; a prime symbol denotes a derivative with respect to x. The system (9) comes from the mass conservation law

$$\dot{c} - vc' + \Omega j' = 0 \tag{12}$$

with

$$Nj = -Bc' - Kc \ ;$$

another consequences of (12) are

$$(C^R - C^{R\times})/\tau - v(c^R - c^{\diamond}) - \Omega j^{\diamond} = 0 \tag{13}$$

and

$$(C^L - C^{L\times})/\tau - v(c^L - c^{\diamond}) - \Omega j^{\diamond} = 0 \tag{14}$$

where the upper indices ^{L} and ^{R} refer to the values at x^L and x^R, respectively. The iterative computational algorithm for any time step, suggested in [34], is based on the solution of the system (9) with B and K estimated from the preceding iterative step, but with respect to the unknown parameters $c^{\diamond}$ and $j^{\diamond}$; v is received by the numerical integration from (11), the results of numerical integration in (10) must be carefully incorporated into (9). The moving boundary conditions are needed for the determination of $c^{\diamond}$ and $j^{\diamond}$ (and consequently of c) from (13) and (14) in each iterative step a posteriori.

The numerical experiments (making use of the original MATLAB- and MAPLE-based software code) with a purely substitutional Fe-rich (q=3, r=0) Fe-Cr-Ni system (whose complete experimental description has been obtained from the Montanuniverität Leoben in Austria and from the Institute of Physics of Materials of the Academy of Sciences of the Czech Republic in Brno) for various fixed temperatures T between 1020 and 1080 K show that for steady-state simulation (neglecting $\dot{c}$ in (12) and the corresponding terms in all remaining relations) predicts some positive constant velocity v decreasing with T. However, the temperature T corresponding to $v \to 0$ is not quite the same as that received for the sharp interface (assuming $h \to 0$); this temperature has been validated indirectly by practical observations. The time-dependent simulation is moreover able to predict the characteristics of the whole process of phase transformation, including the sign changes of v and the possible convergence $v \to 0$ in time. The time distributions of c (at least after some sufficiently long time) are typically nearly constant from the rough view (connected with H), but they can be recognized as rather complicated functions of x in the fine scale (connected with h): this seems to be also the reason why no reference to such other simulation software can be found in the literature.

The above discussed numerical calculations generate reasonable results, but their interpretation using the two-scale (or other) homogenization approach is not available: we were not successful to identify some size parameter with the needed $\varepsilon \to 0$ and the derivation of some relatively simple limit form of our integro-differential problem cannot be expected. This may demonstrate certain limitations of the homogenization techniques, but also motivate their improvements and further development.

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