A Two-Level Approach to Describing the Process of Composite Synthesis

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Article history	Abstract
	The article describes some problems arising in the construction of models of synthesis of composites in modern technologies, which allow predicting the evolution of composition and properties. It is emphasized that the known two-level models practically do not discuss the correspondence between scales and the correctness of information transfer from one level to another, the correctness of computational algorithms requiring the agreement of scales both physical and geometrical. A general approach to building two-level models of synthesis of composites with reinforcing particles based on separation of physical scales is described. It is shown that two-level models of composites synthesis have thermodynamic justification. The variants of estimation of stresses accompanying the change of composition at micro-(meso-)level are proposed. Possible variants of mesolevel submodels for description of composition evolution are briefly presented.

1. INTRODUCTION

Revealing the compliance between the processes occurring in the dynamics during the creation of new materials at different scale levels, including the formation of equilibrium and nonequilibrium chemical compounds and phases, the formation of accompanying and residual stresses and deformations that change the trajectories of chemical state variables, etc., allows us to identify formation mechanisms of structure and properties. However, in the experimental works, as a rule, there is information about the initial materials (mixture), the primary conditions of the experiment and about the final (resulting) products (samples), from which with the help of additional manipulations slips for the study are taken. To solve the related problems, mathematical modeling is actively involved, using both commercial programs and specially developed rather detailed models. Among them, multiphysics modeling and multilevel models play a significant role. Multiscale and multilevel approaches are widespread in materials science [1–3] for modeling the structure and properties of materials and their mechanical behavior, as well as in biophysics [4,5], geophysics [6], mechanics [7,8], etc. Multilevel approaches are also available in

chemistry [9]. Of the three terms used in the literature — *multi-scale, multi-physical* and *multi-level approaches* — the first seems to be the most common, since the same process can proceed at different spatial scales, and different physical processes running together are characterized by different spatial and temporal scales. There are numerous reviews in which the possibilities of multiscale approaches are discussed, their classification is carried out, and thermodynamic and mathematical limitations are established.

However, in application to the processes of synthesis of new materials, including composites with formation of strengthening particles "in situ", complex related models with prognostic properties are rare. The available models practically do not discuss the correspondence between scales and correctness of information transfer from one level to another, correctness of computational algorithms requiring agreement of scales both physical and geometrical. Different simplifications are used to solve arising problems: separation of scales, homogenization, averaging, asymptotic approximations.

A single solution to these problems seems to be impossible, since each specific chemical system has its own peculiarities. Let us focus on the example of synthesis of composites from metal powders with additives of

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elements forming the hardening phase in situ, under laser and electron-beam influence. When developing models and their numerical implementation, there are problems of mathematical and computational nature that require special discussion.

What phenomena are observed in laser and electron-beam fusion of powders [10–12]?

The laser or electron beam travels along the surface to be treated along a specified trajectory; the surface is heated. There is melting of powders of one or more types. A bath of melt and a two-phase zone (where there are solid particles and melt) are formed. The porosity changes. Non-melting particles may disintegrate, dissolve. Heating and melting processes are accompanied by diffusion and chemical reactions. Diffusion can be surface, bulk, at the boundaries of grains and phases, in the solid and liquid phase. Chemical reactions can occur both in volume and at the boundaries. As a result, new phases and compounds are formed, and this, in addition to temperature, leads to changes in properties (both thermophysical and mechanical). Behind the moving melt region there is cooling, crystallization and structure formation; defects appear, secondary porosity is formed. All this is accompanied by the appearance of stresses and deformations of different physical nature, which, in turn, directly or indirectly affect structural and chemical changes. The scale ladder can go down quite deeply [9,13,14]. There are many publications in the literature that model certain processes or stages, with varying degrees of detail. However, there is still a long way to predictive modeling in this area due to the different nature of uncertainties [15,16].

In the present paper we will briefly describe the two-level approach to the construction of the composite synthesis model (Section 2); then we will dwell on the problems arising from the complication of models (Section 3); and finally (Section 4) we will discuss the possible variants of submodels of the evolution of chemical composites in the synthesis process.

2. GENERAL CONSIDERATIONS

During laser or electron-beam scanning of a surface all processes occur simultaneously and can be repeated many times. In our approach we will distinguish two levels and divide all observed processes into two main groups (Fig. 1). The first, directly related to the heating, is the heating of a macro-sample by a moving heat source, accompanied by heat redistribution by thermal conduction, heat loss by convection (mainly in the case of a laser) and radiation. Thermal stresses are linked to inhomogeneous heating. The effective properties of the macro-sample, the total chemical heat release and the stresses of the second kind are considered to be a consequence of the processes
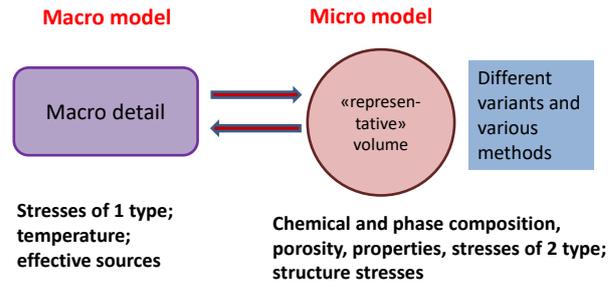
Fig. 1. Illustration to the division of processes according to spatial scales.

of the second group, which lead to changes in the composition and structure and "proceed" at a lower scale level.

That is, as in any multilevel approach based on physical scale separation, the result obtained at one of the levels is either an input parameter for an adjacent level or an initial or boundary condition for it. The approach relies on a macromodel and uses a micromodel to provide missing data. Models at different scales can be quite different in nature and different methods can be used to implement them. However, in both micro (or meso-) and macromodel the need to use homogenization, averaging and asymptotic approximations appears [17–20]. Such an approach also has a thermodynamic justification.

If we have the basic macroscopic state variables Z_k and additional variables ζ_j (generalized basic and additional coordinates), then the basic form of the Gibbs equation can be represented in form

$$du = Tds + B_k dZ_k + \beta_j d\varsigma_j, \qquad (1)$$

where u is the density of internal energy; T is temperature; s is entropy; values B_k and β_j can be regarded as generalized forces corresponding to generalized coordinates. We consider Z_k as components of the strain tensor ε_{ij} conjugated with the Kirchhoff stress tensor, and ς_j as parameters characterizing the composition (volume fractions of phases, which include some or other components). It is follows from Eq. (1) that

$$u = u\left(s, Z_k, \varsigma_j\right).$$

Then

$$B_l = B_l\left(s, Z_k, \varsigma_j\right)$$

and

$$dB_l = \left(\frac{\partial B_l}{\partial s}\right)_{\varepsilon, Z, \xi} ds + \left(\frac{\partial B_l}{\partial Z_k}\right)_{s, \varsigma, Z_i, i \neq k} dZ_k + \left(\frac{\partial B_l}{\partial \varsigma_j}\right)_{s, Z_i, \varsigma_m, m \neq j} d\varsigma_j. \qquad (2)$$

By introducing free energy $f = u - Ts$ instead of Eq. (1) we obtain

$$df = -s\,dT + B_k\,dZ_k + \beta_j\,d\varsigma_j, \tag{3}$$

and instead of Eq. (2)

$$dB_l = -\left(\frac{\partial B_l}{\partial T}\right)_{\varepsilon,Z,\varsigma} dT + \left(\frac{\partial B_l}{\partial Z_k}\right)_{T,\varsigma,Z_i,i\neq k} dZ_k + \left(\frac{\partial B_l}{\partial \varsigma_j}\right)_{T,Z_i,\varsigma_m,m\neq j} d\varsigma_j \tag{4}$$

or

$$d\sigma_{kl} = \left(\frac{\partial \sigma_{kl}}{\partial T}\right)_{\varepsilon,\varsigma} dT + \left(\frac{\partial \sigma_{kl}}{\partial \varepsilon_{\alpha\beta}}\right)_{T,\varsigma} d\varepsilon_{\alpha\beta} + \left(\frac{\partial \sigma_{kl}}{\partial \varsigma_j}\right)_{T,\varepsilon,\varsigma_m,m\neq j} d\varsigma_j. \tag{5}$$

The changes in the components of the stress tensor consist of three parts: changes in the thermal stresses, stress increments related explicitly to the components of the total strain tensor, and stress increments caused by changes in additional state variables. All components, independent of the method of their determination, enter into relations (5) additively. However, the coefficients at the differentials may be functions of all state variables

$$d\sigma_{kl} = A_{kl}(T,\varepsilon,\varsigma)dT + C_{kl\alpha\beta}(T,\varepsilon,\varsigma)d\varepsilon_{\alpha\beta} + B_{kl,j}(T,\varepsilon,\varsigma)d\varsigma_j. \tag{6}$$

All values depend on spatial coordinates x, y, z and time t.

By definition, the additional variables evolve according to some laws that work at the lowest scale level, where one can introduce one's own (internal or local) coordinate system. Generally speaking, the equation of state similar to Eq. (6) takes place for the lowest scale level. But since we have divided physical processes by scales, we need to establish compliance between microscale variables and macroscale variables responsible for composition changes.

We will assume that

$$\varsigma_j = \langle Y_j \rangle, \tag{7}$$

where

$$Y_j = Y_j(x,y,z;x',y',z',t) = Y_j(\mathbf{R};\mathbf{r},t), \tag{8}$$

$\mathbf{R}$ is radius-vector of a point in the macroscale coordinate system; $\mathbf{r}$ is the radius-vector of the coordinate system on the microscale.

3. PROBLEMS

The decision to use a multiscale approach implies a compromise between the increased predictive power of the model and the additional complexity of internal relationships, and between the corresponding decrease in computational accuracy and the increase in uncertainty that multiscale modeling brings [21]. Moreover, there is no rigorous proof of the correctness of transitions between scale levels, which is hidden behind the accepted hypotheses. The two-level approach to modeling the synthesis of composites, which was actively developed in macrokinetics in the 1970s–80s, is not devoid of these problems [22–25]. On the one hand, the models clearly show the scale of the heterogeneous structure and the diffusion mechanism of the reaction involving refractory reactants and/or reaction products; on the other hand, the necessity of applying the hypothesis of the correspondence of the sequence of stages to equilibrium state diagrams appears. Both in the first works resorting to the notion of reaction cells and in the later ones [26–30], the reaction kinetics proper, the diffusion mechanisms in different phases and on the surface, and the particle structure playing an important role in the evolution of phase and chemical composition are not discussed. Problems related to the interaction of diffusion and chemical stages with their accompanying mechanical stresses also remain without attention. Let us outline some other problems that have also appeared in simpler situations when trying to combine different-scale processes or the evolution of properties during synthesis and processing.

A variant of the two-level model of composite surface machining with an explicit description of the formation of the transition zone between inclusions and matrix is presented in Ref. [31]. It is assumed that in each section of the heterogeneous material $z = z_0 = 0$; z_1; z_2; ..., parallel to the machined surface and having a temperature $T_s = T(0,t)$; $T_1 = T(z_1,t)$; $T_2 = T(z_2,t)$; ..., respectively, the particles are in different conditions, depending on the heating rate, which follows from the solution of the "macro" thermal problem. The assumption of smallness of the particles is used. A conjugate diffusion problem for the formation of a transition zone between the particle and the matrix is solved at each cross section. On the basis of this model, the difference in the dynamics of temperature changes and in the character of transition zone formation for particles located at different depths from the surface layer, depending on the irradiation regime, is analyzed.

In the evaluation of mechanical stresses in the processed composite [32], the change in the composition and properties of the matrix in the vicinity of the particles was taken into account. However, the effect of stresses on diffusion was not analyzed; the change in the mechanical properties of the matrix with the appearance of an alloying element in its composition was accounted for by the mixture rule, which requires, of course, additional justification. A similar approach to taking into account the composite structure when describing melting is used in much later work [33].

The same problem arises when the temperature dependence of the properties is taken into account. Taking

into account the dependence of properties on temperature leads to a change in the results. For example, in the thermophysical model of part surface modification by scanning electron beam [34] it is shown that taking into account the dependence of thermal conductivity coefficient on temperature leads to changes both in the temperature itself and in the time of establishing a quasi-stationary regime, the size and shape of the melt bath and thermal influence zone. The problem is that if there is a change in the chemical composition in the process of modification, such dependences are unknown for many materials.

One of the goals of modeling electron beam or laser modification of surfaces is to estimate the effective properties of the formed materials and coatings. In micromechanics [35], this problem is solved using different approaches. But, as a rule, it is assumed that the composite structure as well as the composition and properties of the phases are known in advance; the evaluation of the effective properties is performed according to the data on the structure and composition obtained from the experiment. However, in the process of synthesizing a new material, the properties are continuously changing (depending on temperature and composition; the specific structure at any given time is unknown). The question arises: "Which of the known methods of property estimation is correct to use in this case"? In the same model with the addition of inert particles, it was proposed to determine the possible area of change of properties by the beam [34]. However, in the simulation of the actual process of cladding and surface treatment, the change of properties with composition and temperature was not analyzed.

Note, in some works, when estimating the area of change in the effective properties of materials, the authors formally calculate the heat capacity in the same way as the thermal conductivity, using the formulae

$$\lambda_{eff} = \sum_{(k)} \lambda_k \xi_k, \quad c_{eff}\rho_{eff} = \sum_{(k)} c_k \rho_k \xi_k, \quad (9)$$

or

$$\frac{1}{\lambda_{eff}} = \sum_{(k)} \frac{\xi_k}{\lambda_k}, \quad \frac{1}{c_{eff}\rho_{eff}} = \sum_{(k)} \frac{\eta_k}{c_k \rho_k}. \quad (10)$$

However, heat capacity, by definition, is an additive quantity. It does not depend on the structure. It only depends on the composition. Indeed, by definition

$$C = T\left(\frac{\partial S}{\partial T}\right),$$

if any thermodynamic force or thermodynamic coordinate (such as pressure or volume) and all other quantities, such as composition, are constant.

When a thermodynamic system consists of parts with volume fractions ξ_k, then

$$S = \sum_{(k)} S_k \xi_k.$$

Hence

$$C = T\left(\frac{\partial \sum_{(k)} S_k \xi_k}{\partial T}\right) = \sum_{(k)} C_k \xi_k. \quad (11)$$

The derivatives here must be taken when the composition is constant. So only formulas (9) are valid for heat capacity. This is not true in the non-additive thermodynamics of Tsallis.

An attempt to use methods of micromechanics to estimate the properties of composites during their synthesis was made in Refs. [36,37].

In Ref. [38] and others, the structure of the material as a result of electron beam alloying is also judged, as in Refs. [32,34], by the history of temperature changes, the calculation of which, however, does not take into account possible changes in composition and structure, leading to a change in properties. A similar approach to the modeling of structure formation in the selective laser melting process is used by the authors of various works [39–41]. Such two-level models can be called sequential: i.e., in order to move to the next level, it is necessary to obtain all the information from the previous level.

However, there is another problem here. The temperature field is calculated in the quasi-stationary approximation [42,43]. The authors implicitly assume that such a quasi-stationary regime is necessarily realized in the corresponding 3D technologies. Then, knowing the temperature and temperature gradients in different parts of the computational domain, they say which structure and which phases should be realized. Almost all authors proceed from the statement that these processes are similar to welding. None of these works takes into account the influence of the changing structure on the properties appearing in the heat conduction problem. There is no justification for the choice of characteristic points at which the structure is analyzed. There is no justification for the accepted fact that it is always possible to identify a characteristic quasi-stationary melt bath and typical temperature curves. Examples of the fact that the quasi-stationary regime may not be realized at all or may be different for different points of the macro sample are contained in Refs. [44–46].

Often, using commercial software packages, the authors do not bother to write down a correct formulation of the problem. And the most interesting thing is that everything agrees well with the experiment. In fact, in Ref. [42] the heat conduction problem with boundary conditions which take into account all kinds of heat exchange and with a complicated dependence of heat transfer coefficient on temperature is solved (the authors pretend to take into

account different mechanisms of heat exchange) and in Ref. [43] the method of lattice Boltzmann equations is used. The authors do not give a clear statement and description of all approximations.

The next problem is related to the description of melting in a complex system. There are different variants in the literature. The simplest one is to set a certain effective melting temperature; the corresponding heat losses are taken into account as a sharp increase in heat capacity at this temperature. For simple (single-component) systems, this approach quite reflects the real laws. But if the system consists of several components (for example, powders of different metals), then (A) it is possible to introduce a different melting temperature for each type of powder in Eq. (11)

$$C = \sum_{(k)} C_k \xi_k, \quad C_k = C_{k0} + L_k \delta(T - T_{mk}),$$

where T_{mk} and L_k are temperatures and melting heats of the components; $\delta(T - T_{mk})$ is Dirac delta function.

Another option (B): two melting temperatures — minimum T_{min} and maximum T_{max} — are introduced in the system. Between these temperatures, the fraction of the liquid phase η_L changes according to some system-dependent law, e.g:

$$\eta_L = \begin{bmatrix} 0, & T < T_{min}; \\ \left(\dfrac{T - T_{min}}{T_{max} - T_{min}}\right)^n, & T_{min} \leq T < T_{max}; \\ 1, & T \geq T_{max}. \end{bmatrix}$$

This is, in a way, an analogue of the two-phase zone theory. The law of liquid phase accumulation can also be set for each type of powder.

How do we distinguish between solidification and crystallization in this case? Intermetallic phases stand out as phases (i.e., regions with some composition and corresponding structure) on cooling. Do they exist at higher temperatures as individual chemical compounds in solution? Or is it problematic to isolate such compounds? Apparently, as in reactive diffusion models, an explicit isolation of diffusants responsible for the diffusion mechanism of phase formation at lowering temperature is required. But the rates and scales of diffusion processes in solid phases are much smaller than the scales and speeds of the thermal conductivity process, which does not allow us to hope for explicit accounting within a single model of diffusion-kinetic phenomena without the introduction of additional assumptions.

Attempts to describe the melting process of a two-component powder using filtration theory are interesting [47,48]. However, there are doubts about the applicability of Darcy's law to a region consisting of 3–10

powders and the melt flowing around them (typical size of the melting zone in laser 3D technology).

Perhaps the most serious problem is related to the adequate description of chemical transformations under conditions of laser and electron beam 3D technologies. There are publications with information on the synthesis of intermetallic and metal matrix composites using these technologies [49–51]. The reactions that take place are essentially heterogeneous; either one of the reactants is solid or the reaction product is solid. In powder media, chemical reactions proceed at the particle scale level. The problem of modeling physicochemical transformations involving solids is not new and finds a variety of solutions in solid-state chemistry and continuum mechanics. The following can be added to the features already mentioned [52]. Because of the low mobility of components, reactions localize at and near interfaces. Most reactions involving solids are macrokinetic processes; that is, the reaction stages are different physical processes. Because of the heterogeneous distribution of components, reaction rates are also heterogeneous; a variety of kinetic difficulties can lead to significantly different reaction pathways than those expected from thermodynamic considerations. Reactions and their accompanying transfer processes are accompanied by mechanical stresses, defect formation, and destruction, which can also lead to changes in reaction pathways.

One of the ways to describe chemical reactions in complex media that has long been used in macrokinetics is a formal description with the introduction of the degree of transformation (or conversion level). The fraction of reaction product or degree of transformation satisfies the kinetic equation

$$\frac{d\eta}{dt} = k_0 \phi(\eta) \exp\left(-\frac{E}{RT}\right).$$

The type of the kinetic function depends on the processes occurring at the microlevel. Special problems are solved to determine them. The activation energy is determined by the activation energy of the limiting stage. The pre-exponent depends on many factors that are not taken into account explicitly and are difficult to reproduce and poorly controllable in the experiment. The resulting parameters are inconsistent and ambiguous. Nevertheless, this approach is very successful and makes it possible to distinguish different modes of product formation.

For some of the systems, the complex of reactions leading to the formation of the composition can be described by two total parallel or sequence-parallel reactions, one of which leads to the formation of the strengthening particle material and the other to the formation of the matrix [53,54]. Such a formal scheme is acceptable when describing the synthesis of composites from mixtures of Ti-Al-C; Ti-Al-B; Ti-Al-Fe$_2$O$_3$; Al-Fe$_2$O$_3$-Fe-Cr-

Ni; Ti-Fe$_2$O$_3$-Nb, etc. For example, in a mixture of Ti-Al-C powders, titanium and carbon are consumed to form carbide particles as well as to form the matrix. That is, the same reagent is consumed in two parallel reactions running at different rates. In the system Ti-Al-Fe$_2$O$_3$ particles are formed by metallothermic reaction, and the product of this reaction (Fe) takes part in matrix formation. I.e., in this case we have a system of series-parallel total reactions. Both reactions are exothermic. A similar scheme is correct for the Al-Fe$_2$O$_3$-Fe-Cr-Ni system, but the second of the reactions may also be cumulatively endothermic. The intermediate product may be present in the mixture initially. However, this is not sufficient to explain the physical mechanisms of composite structure formation and predict their properties.

The use of a more or less detailed scheme of chemical transformations with the introduction of a special kind of kinetic functions, taking into account the inhibition of reactions by a layer of solid-phase products [55], allows us to predict the composition of synthesis products, but requires finding or selecting in accordance with experimental data a set of formal and kinetic parameters, which is solved ambiguously.

4. POSSIBLE VARIANTS OF PHASE FORMATION MODELS

In general thermodynamics, phase- and structure-formation processes are modeled differently. For example, chemical variables (reaction coordinates, component concentrations) can be considered as variables leveled with others [56,57]. In some situations, some internal variables [58,59], the evolution of which affects the behavior of the main variables, can also be considered chemical variables. As order parameters, chemical variables appear in the phase-field method theory [60]. Using the splitting of processes by values of characteristic temporal and spatial scales (Fig. 1), let us analyze some possible variants of micro-(meso)level models.

For example, in a mixture of xTi+yAl+zCuO powders, the reduction of copper from oxide is thermodynamically possible:

$3CuO + 2Al \rightarrow 3Cu + Al_2O_3$,

$Ti + 2CuO = TiO_2 + 2Cu$.
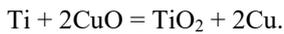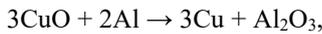
Obviously, these are total reactions; in fact, they include several stages and can occur in both liquid and solid phases. Of the starting substances, Al has the lowest melting point (933 K). This is followed by copper oxide (1716 K). The most refractory is titanium (1943 K).

If titanium is in excess, phases Cu$_4$Ti, Cu$_3$Ti$_2$, TiCu$_2$, Cu$_4$Ti$_3$, CuTi, CuTi$_2$, CuTi$_3$ may appear. If aluminum is in excess, we can assume intermetallide formation reactions

$Al + Cu = AlCu$,

$AlCu + Al = Al_2Cu$ et al.
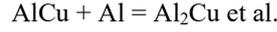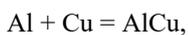
Since metallothermic reactions proceed with a significant thermal effect, it is logical to assume that once aluminum melts and the reduction reaction begins, the process most likely proceeds in the liquid phase.

The following variants of two-level models of synthesis of composites are possible, in which the composition of the composite is determined at the microlevel. In accordance with Ref. [61], in numerical implementation of such models, at each step of macro-problem solution the micro-problem can be considered in quasi-stationary approximation.

(A) Based on the selection of conditional or equivalent mesocells with movable boundaries between phases of different composition. For binary mixtures of Al-Ti, Al-CuO, and Ti-CuO, variants of reaction cells similar to combustion theory models can be proposed, assuming that a refractory particle is located in the center of the cell. However, the size of the conditional solid spherical particle may clearly not correspond to the size of the powder particles. In a mixture of three types of particles, such conditional reaction cells can be taken with weights β_k depending on the initial concentration of components and the ratio of powder sizes. At each point of a macro sample, the composition in the cell of each type is determined from the solution of the reaction diffusion problem. The new phases are more refractory than the initial phases, so that diffusion through the product layers clearly slows their growth. The average composition in each point is

$$\varsigma_j = \sum_{(k)} \beta_k \left\langle Y_{j,k} \right\rangle, \tag{11}$$

where $Y_{j,k}$ is a fraction of jth phase in kth cell. At the level of each cell, it is possible to determine both the fractions of the phases bounded by the interfaces and the distribution of the components in the phases at the current moment in time.

The associated stresses and strains in the two-level model can be "estimated" in two ways. The first option is reduced to solving the problem of mechanical equilibrium in each cell, the consequence of which will be the components of the stress and strain tensors in the spherical coordinate system. Using the averaging procedure and passing to the macroproblem coordinate system, we find stresses of the second kind, which we sum up with the stresses of the first kind found when solving the mechanical equilibrium problem at the macrolevel. Thus,

$$\sigma_{ij} = \sigma_{ij}^M + \sigma_{ij}^T + \sigma_{ij}^C, \tag{12}$$

where σ_{ij}^M are the stresses associated directly with reversible strains, stresses $\sigma_{ij}^T = \sigma_{ij}^I$ are calculated in the macro task, and stresses $\sigma_{ij}^C = \sigma_{ij}^{II}$ are the result of averaging solutions for meso-(micro) volumes.

In the second variant, the mechanical equilibrium problem uses the composition obtained from the solution of the microtask and the defining relations of the form (6). However, the influence of accompanying stresses on diffusion and reaction rates (i.e., transition to a coupled model) can be taken into account only in the first variant.

(B) Based on the phase field method and its generalization at each point of a macro sample at the temperature of that point, the problem of determining the equilibrium composition is solved. The problem is how to determine the structure and size of a representative volume. Will the result depend on its shape? None of the papers that use the phase-field method to determine composition and structure from temperature evolution data discuss this question and require separate consideration. Related models of composite synthesis based on this approach have not been discussed in the literature, but they can be formulated similarly to option (A).

(C) At each point of a macro sample, we analyze the problem of composition evolution in a multiphase and multicomponent mesovolume, considering the exchange of components between phases, evolution of porosity, flow in pores, appearance of new phases and accompanying stresses. In this application similar models of composites synthesis are also absent in literature.

A comparison of the three versions of the evolution of composition will make it possible to develop an approach to the construction of two-level models with the best predictive power.

5. CONCLUSION

Thus, the mathematical and physical problems arising in the construction of models of synthesis of composites applicable to modern technologies require careful attention and cannot be solved in a general way. Different types of systems, characterized by different initial compositions, under non-equilibrium synthesis conditions undergo changes that cannot be predicted on the basis of traditional approaches. Two-level models of synthesis of composites have thermodynamic justification, but among the possible variants of mesolevel sub-models to describe the evolution of composition and variants of evaluation of stresses accompanying changes in composition and structure and affecting the course of transformations, there are not yet those that would allow predicting composition, structures and properties under changing technological conditions.

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Двухуровневый подход к описанию процесса синтеза композитов

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Аннотация. В статье перечислены некоторые проблемы, возникающие при построении моделей синтеза композитов, позволяющих прогнозировать эволюцию состава и свойств в и применимые к современным технологиям. Подчеркивается, что в известных двухуровневых моделях практически не обсуждается соответствие между масштабами и корректность передачи информации с одного масштабного уровня на другой, корректность вычислительных алгоритмов, требующих согласования масштабов как физических, так и геометрических. Описан общий подход к построению двухуровневых моделей синтеза композитов с армирующими частицами, основанный на разделении физических масштабов. Показано, что двухуровневые модели синтеза композитов имеют термодинамическое обоснование. Предложены варианты оценки напряжений, сопровождающих изменение состава на микро- (мезо-) уровне. Кратко представлены возможные варианты подмоделей мезоуровня для описания эволюции состава.

Ключевые слова: синтез композита; двухуровневый подход; сопутствующие напряжения; подмодели