

Chapter 2

General Equations of Multiphase Continuum Mechanics for Ablative Composites

Abstract Models of multiphase media mechanics have been considered in many works [1–14, 16–28, 30–34, etc.]. In the present chapter general relationships of multiphase media mechanics are developed for ablative composites. These are the key points: derivation of expressions for a phase transformation rate with the help of thermodynamical equations at a phase interface; and determination of the way in which constitutive relations depend on the characteristics of the natural configurations of phases. In the first four paragraphs the general case of finite deformations of phases is considered using, in the main, the Euler (space) description given in works [6, 16, 29, etc.]; and in the last paragraph the case of infinitesimal deformations of phases is analyzed.

2.1 Conservation Laws

2.1.1 Main Concepts of Tensor Analysis

Consider the motion of a continuum in the Cartesian coordinate system $O\mathbf{x}$ with basis vectors $\mathbf{e}_k$, $k = 1, 2, 3$. The geometrical location of the medium at the initial time $t = 0$ in the coordinate system is called the *initial configuration* $\overset{\circ}{V}$, and at time $t > 0$ —the *actual configuration* $V(t)$ (see [16]).

Let radius-vectors of a material point in the actual $V(t)$ and initial $\overset{\circ}{V}$ configurations be $\mathbf{x} = x^k \mathbf{e}_k$ and $\overset{\circ}{\mathbf{x}} = \overset{\circ}{x}^k \mathbf{e}_k$, respectively, where x^k and $\overset{\circ}{x}^k$ are the coordinates of the same material point M in configurations V and $\overset{\circ}{V}$. Introduce the *material coordinates* X^k individualizing the material point M . Motion of the medium is described by the equations $\mathbf{x} = \mathbf{x}(X^k, t)$; location of a material point with coordinates X^k in the initial configuration is determined by the equations

$$\overset{\circ}{\mathbf{x}} = \overset{\circ}{\mathbf{x}}(X^k).$$

Indices $k, s, p, r, \dots$ here and below are indicators of components of tensors and take the values 1, 2, 3; summation from 1 to 3 is denoted by a repeated index.

Introduce vectors $\mathbf{r}_k$ of a *general local basis* and vectors $\mathbf{r}^k$ of a *coupling local basis* in the actual configuration, and vectors $\overset{\circ}{\mathbf{r}}_k$ and $\overset{\circ}{\mathbf{r}}^k$ in the initial configuration, respectively [16]:

$$\begin{aligned}\mathbf{r}_k &= \frac{\partial \mathbf{x}}{\partial X^k} = \frac{\partial x^s}{\partial X^k} \mathbf{e}_s, & \overset{\circ}{\mathbf{r}}_k &= \frac{\partial \overset{\circ}{\mathbf{x}}}{\partial \overset{\circ}{X}^k} = \frac{\partial \overset{\circ}{x}^s}{\partial \overset{\circ}{X}^k} \mathbf{e}_s, \\ \mathbf{r}^k &= \frac{\partial X^k}{\partial x^s} \mathbf{e}_s, & \overset{\circ}{\mathbf{r}}^k &= \frac{\partial \overset{\circ}{X}^k}{\partial \overset{\circ}{x}^s} \mathbf{e}_s.\end{aligned}$$

The concept of the *dyad* [15, 16] of vectors $\mathbf{a}$ and $\mathbf{b}$ is introduced, and denoted by $\mathbf{a} \otimes \mathbf{b}$. With the help of dyads $\mathbf{r}^k \otimes \mathbf{r}^s$, $\mathbf{r}_k \otimes \mathbf{r}_s$, $\overset{\circ}{\mathbf{r}}^k \otimes \overset{\circ}{\mathbf{r}}^s$ of the vectors of the local basis and others, or of the Cartesian basis $\mathbf{e}^k \otimes \mathbf{e}^s$, we may form *dyadic bases*; then each second-order tensor $\mathbf{A}$ can be written in the form

$$\mathbf{A} = A^{sk} \mathbf{r}_s \otimes \mathbf{r}_k = A_{sk} \mathbf{r}^s \otimes \mathbf{r}^k = A_k^s \mathbf{r}_s \otimes \mathbf{r}^k = \overset{\circ}{A}^{sk} \overset{\circ}{\mathbf{r}}_s \otimes \overset{\circ}{\mathbf{r}}_k,$$

where A^{sk} , A_{sk} , A_k^s are respectively the *contravariant*, *covariant* and *combined components* of the tensor $\mathbf{A}$, in the corresponding dyadic basis.

Scalar products of vectors of the local bases have the forms

$$\begin{aligned}\mathbf{r}_k \cdot \mathbf{r}_s &= g_{ks}, & \mathbf{r}^k \cdot \mathbf{r}^s &= g^{ks}, & \mathbf{r}_k \cdot \mathbf{r}^s &= g_k^s = \delta_k^s, \\ \overset{\circ}{\mathbf{r}}_k \cdot \overset{\circ}{\mathbf{r}}_s &= \overset{\circ}{g}_{ks}, & \overset{\circ}{\mathbf{r}}^k \cdot \overset{\circ}{\mathbf{r}}^s &= \overset{\circ}{g}^{ks}, & \overset{\circ}{\mathbf{r}}_k \cdot \overset{\circ}{\mathbf{r}}^s &= \overset{\circ}{g}_k^s = \delta_k^s,\end{aligned}$$

where δ_k^s is the *Kronecker symbol*, g_{ks} and $\overset{\circ}{g}_{ks}$ are the components of the *metric (unit) tensor* $\mathbf{E}$ in the configurations V and $\overset{\circ}{V}$, respectively. The tensor E is determined as follows:

$$\begin{aligned}\mathbf{E} &= \mathbf{r}^k \otimes \mathbf{r}_k = g^{ks} \mathbf{r}_k \otimes \mathbf{r}_s = g_{ks} \mathbf{r}^k \otimes \mathbf{r}^s \\ &= \overset{\circ}{\mathbf{r}}^k \otimes \overset{\circ}{\mathbf{r}}_k = \overset{\circ}{g}^{ks} \overset{\circ}{\mathbf{r}}_k \otimes \overset{\circ}{\mathbf{r}}_s = \overset{\circ}{g}_{ks} \overset{\circ}{\mathbf{r}}^k \otimes \overset{\circ}{\mathbf{r}}^s = \mathbf{e}_k \otimes \mathbf{e}^k.\end{aligned}$$

Passage from the general basis vectors to the coupling basis vectors is realized with the help of the components g^{ks} and $\overset{\circ}{g}^{ks}$:

$$\begin{aligned}\mathbf{r}^k &= g^{ks} \mathbf{r}_s, & \mathbf{r}_k &= g_{ks} \mathbf{r}^s, \\ \overset{\circ}{\mathbf{r}}^k &= \overset{\circ}{g}^{ks} \overset{\circ}{\mathbf{r}}_s, & \overset{\circ}{\mathbf{r}}_k &= \overset{\circ}{g}_{ks} \overset{\circ}{\mathbf{r}}^s.\end{aligned}$$

Scalar products of vector $\mathbf{a}$ and tensor $\mathbf{A}$, and also tensors $\mathbf{A}$ and $\mathbf{B}$ with respect to one or two indices are determined as follows:

$$\mathbf{a} \cdot \mathbf{A} = a^k A_{ks} \mathbf{r}_s, \quad \mathbf{A} \cdot \mathbf{B} = A^{kr} B_{rs} \mathbf{r}_k \otimes \mathbf{r}^s, \quad \mathbf{A} \cdot \cdot \mathbf{B} = A^{ks} B_{sk},$$

where

$$\mathbf{B} = B^{sk} \mathbf{r}_s \otimes \mathbf{r}_k, \quad \mathbf{a} = a^k \mathbf{r}_k.$$

Tensor and vector products of vector $\mathbf{a}$ and tensor $\mathbf{A}$ are defined by the formulae

$$\mathbf{a} \otimes \mathbf{A} = a^k A^{rs} \mathbf{r}_k \otimes \mathbf{r}_r \otimes \mathbf{r}_s, \quad \mathbf{a} \times \mathbf{A} = \sqrt{g} \epsilon_{ksp} a^k A^{sr} \mathbf{r}^p \otimes \mathbf{r}_r,$$

here $\mathbf{r}_k \otimes \mathbf{r}_r \otimes \mathbf{r}_s$ is the *triad* of the local basis vectors, $g = \det(g_{sk})$ is the determinant of the *metric matrix* and ϵ_{ksp} are the *Levi-Civita symbols*.

The *inverse tensor* $\mathbf{A}^{-1}$ and *transpose tensor* $\mathbf{A}^T$ are defined as follows:

$$\mathbf{A} \cdot \mathbf{A}^{-1} = \mathbf{E}, \quad \mathbf{A}^T = A^{sk} \mathbf{r}_k \otimes \mathbf{r}_s.$$

Sequential application of the inversion and transposition to tensor $\mathbf{A}$ gives the *inverse-transpose tensor* $\mathbf{A}^{-T}$:

$$(\mathbf{A}^{-1})^T = (\mathbf{A}^T)^{-1} = \mathbf{A}^{-T}.$$

The differential *Hamilton nabla-operator* ∇ of the scalar θ , vector $\mathbf{a}$ and tensor $\mathbf{A}$ in the initial configuration are determined as follows:

$$\begin{aligned} \nabla \theta &= \mathbf{r}^k \frac{\partial \theta}{\partial X^k} = \frac{\partial \theta}{\partial x^k} \mathbf{e}_k, \quad \nabla \cdot \mathbf{a} = \mathbf{r}^k \cdot \frac{\partial \mathbf{a}}{\partial X^k} = \frac{\partial \mathbf{a}}{\partial x^k} \cdot \mathbf{e}_k, \\ \nabla \otimes \mathbf{a} &= \mathbf{r}^k \otimes \frac{\partial \mathbf{a}}{\partial X^k} = \mathbf{e}_k \otimes \frac{\partial \mathbf{a}}{\partial x^k}, \quad \nabla \cdot \mathbf{A} = \mathbf{r}^k \cdot \frac{\partial \mathbf{A}}{\partial X^k} = \mathbf{e}_k \cdot \frac{\partial \mathbf{A}}{\partial x^k}, \\ \nabla \times \mathbf{A} &= \mathbf{r}^k \times \frac{\partial \mathbf{A}}{\partial X^k} = \mathbf{e}_k \times \frac{\partial \mathbf{A}}{\partial x^k}. \end{aligned}$$

We will apply these definitions to a continuum, the physical features of which at passage from one material point to another do not change or change continuously. If the functions describing physical properties of continuum are disconnected in the domain V , then the medium is called *composite*.

Suppose that, at time $t > 0$ the domain $V(t)$ of the composite consists of n subdomains, each of which is a physically *homogeneous* medium and called a *phase* of the composite. Each i th phase of the composite occupies a domain $\overset{\circ}{V}_i$ in the initial configuration and $V_i(t)$ in the actual configuration. Let the interface between phases i and j be Σ_{ij} . Here and below indices i and j run over letter values $\{a, b, p, g, l\}$ and correspond to certain phases, and $n = 5$. There is no summation over repeated indices i and j .

We assume the following:

- phase $i = a$ is an amorphous phase of the reinforcing filler;
- phase $i = b$ is a polymer phase of the matrix;

- phase $i = p$ is a pyrolytic phase of the matrix;
- phase $i = g$ is gaseous products of pyrolysis in pores of the composite;
- phase $i = l$ is a crystalline phase of the reinforcing filler.

The transformation of a local vicinity of a material point M from domain V_i into domain V_j at time $t = t_*$ is called a *phase transformation* of the type ' $i \rightarrow j$ '.

For a multiphase medium, in addition to configurations $V(t)$ and $\overset{\circ}{V}$ there also exists an undeformed configuration $\overset{\circ}{V}(t)$ which differs from $\overset{\circ}{V}$ only in that boundaries of domains $\overset{\circ}{V}(t)$ of phases change according to the changing domains $V_i(t)$ therein, and $\overset{\circ}{V}(0) = \overset{\circ}{V} = V(0)$. When phase transformations are absent $\overset{\circ}{V}(t) = \overset{\circ}{V}$.

Within the domains $V_i(t)$, all functions $\overset{\circ}{\mathbf{x}}$, $\mathbf{x}$, $\mathbf{r}_k$, $\overset{\circ}{\mathbf{r}}_k$ and others describing a state of the composite have continuous partial derivatives with respect to x^k and t for all requested orders.

The *displacement vector* $\mathbf{u}_i(x^k, t)$ for material point M , at time t and point $x^k \in V_i(t)$, is determined as follows

$$\mathbf{u}_i(x^k, t) = \mathbf{x} - \overset{\circ}{\mathbf{x}}(X^s(x^k, t)), \quad x^k \in V_i(t).$$

Let us introduce the *strain gradient* $\mathbf{F}_i$, being an unsymmetric second-order tensor

$$\mathbf{F}_i = \mathbf{r}_s(x^k, t) \otimes \overset{\circ}{\mathbf{r}}^s(X^s(x^k, t)), \quad x^k \in V_i(t),$$

which transforms local basis vectors and infinitesimal elements of radius-vectors $d\mathbf{x}$ and $d\overset{\circ}{\mathbf{x}}$ from the initial configuration to the actual one:

$$\mathbf{r}_s = \mathbf{F}_i \cdot \overset{\circ}{\mathbf{r}}_s, \quad d\mathbf{x} = \mathbf{F}_i \cdot d\overset{\circ}{\mathbf{x}} \quad x^k \in V_i(t).$$

The inverse strain gradient $\mathbf{F}_i^{-1}$ is expressed by the formula

$$\mathbf{F}_i^{-1} = \overset{\circ}{\mathbf{r}}_s \otimes \mathbf{r}^s = \frac{\partial \overset{\circ}{x}^s(X^p(x^k, t))}{\partial x^r} \mathbf{e}_s \otimes \mathbf{e}_r, \quad x^k \in V_i(t).$$

2.1.2 System of Conservation Laws for Phases

On the base of relationships given in Sect. 2.1.1 we derive the connection between the inverse strain gradient $\mathbf{F}_i^{-1}$ and the displacement vector $\mathbf{u}_i$

$$\mathbf{F}_i^{-1T} = \mathbf{E} - \nabla \otimes \mathbf{u}_i. \quad (2.1)$$

In the domain V_i occupied by the i th phase, there is a set of *conservation equations for continuum mechanics* which can be written as follows:

$$\frac{\partial \rho_i A_{i\zeta}}{\partial t} + \nabla_x \cdot (\rho_i \mathbf{v}_i A_{i\zeta} - B_{i\zeta}) = C_{i\zeta}, \quad (2.2)$$

$$\mathbf{x} \in V_i, \quad i = a, b, p, g, l, \quad \zeta = 1, \dots, 6.$$

Here $A_{i\zeta}$, $B_{i\zeta}$ and $C_{i\zeta}$ are generalized vectors with the following components:

$$A_{i\zeta} = \begin{pmatrix} 1 \\ \mathbf{v}_i \\ e_i + \frac{v_i^2}{2} \\ \eta_i \\ \mathbf{u}_i \\ \mathbf{F}_i \end{pmatrix}, \quad B_{i\zeta} = \begin{pmatrix} 0 \\ \boldsymbol{\sigma}_i \\ \boldsymbol{\sigma}_i \cdot \mathbf{v}_i - \mathbf{q}_i \\ -\mathbf{q}_i / \theta_i \\ 0 \\ \rho_i \mathbf{F}_i^T \otimes \mathbf{v}_i \end{pmatrix}, \quad C_{i\zeta} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{W_i^*}{\theta_i} - \frac{\mathbf{q}_i \cdot \nabla \theta_i}{\theta_i^2} \\ \rho_i \mathbf{v}_i \\ 0 \end{pmatrix}, \quad (2.3)$$

where $i = a, b, p, g, l$.

Equation system (2.2) consists of

- $\zeta = 1$ —scalar *equation of continuity* for the i th phase;
- $\zeta = 2$ —vector *equation of momentum* for the i th phase;
- $\zeta = 3$ —scalar *equation of energy* for the i th phase;
- $\zeta = 4$ —scalar *equation of entropy balance* for the i th phase;
- $\zeta = 5$ —vector *kinematic equation* for the i th phase;
- $\zeta = 6$ —tensor *equation of strain compatibility* for the i th phase.

In Eqs. (2.2) there are the following notations: ρ_i is the density, $\mathbf{v}_i$ is the velocity, $\boldsymbol{\sigma}_i$ is the stress tensor (also called *Cauchy's stress tensor* or true stress tensor), e_i is the internal energy, $\mathbf{q}_i$ is the heat flux vector, η_i is the entropy, θ_i is the temperature, W_i^* is the energy dissipation function of the composite phases ($W_i^* \geq 0$), $\mathbf{F}_i$ is the strain gradient, $\mathbf{u}_i$ is the displacement vector and $v_i = \mathbf{v}_i \cdot \mathbf{v}_i$. It should be noted that terms of density of internal energy, vector of heat flux density etc. are often used for functions e_i , η_i , $\mathbf{q}_i$ and W_i^* , and terms of internal energy, heat flux vector etc. are applied for integral values averaged over volumes or surfaces of phases. However when one has no need to use the integral values, the word 'density' can be omitted for brevity.

The *conservation laws* set (2.2) has a *divergent form*. Nine scalar equations of strain compatibility in the system at $\zeta = 6$ are equivalent to nine relationships (2.1), and can be used instead of them. Compatibility equations in the divergent form were derived from these relationships for example in [16].

2.1.3 Relationships on a Surface of a Strong Discontinuity

The interface Σ_{ij} between the i th and j th phases at phase transformation is a *singular surface of a strong discontinuity* [16], i.e. when passing through the surface, some of

the functions describing the motion of the composite have discontinuities. Values of an arbitrary function $\Omega_i(\mathbf{x}, t)$ at the singular surface Σ_{ij} are determined by passing to the limit from the side of corresponding phase, V_i or V_j :

$$\Omega_i(\mathbf{x}, t)|_{\mathbf{x} \in \Sigma_{ij}} = \lim_{\substack{\mathbf{x}' \rightarrow \mathbf{x} \\ \mathbf{x}' \in V_i}} \Omega_i(\mathbf{x}', t).$$

The difference between the function values Ω_i and Ω_j at the phase interface Σ_{ij} is called the *jump of a function*:

$$[\Omega] = \Omega_i|_{\mathbf{x} \in \Sigma_{ij}} - \Omega_j|_{\mathbf{x} \in \Sigma_{ij}}. \quad (2.4)$$

For the generalized vectors of the set (2.2) at the phase interface Σ_{ij} , the following jump conditions of the functions hold:

$$[\rho(D - \mathbf{v} \cdot \mathbf{n})A_\zeta + \mathbf{n}B_\zeta] = H_\zeta, \quad \zeta = 1, \dots, 6, \quad \mathbf{x} \in \Sigma_{ij}. \quad (2.5)$$

In the relations (2.5) there are some notations: $\mathbf{n}$ is the normal vector to the surface Σ_{ij} , being external with respect to the j th phase; D is the *speed of the phase interface*; and H_ζ is the generalized vector having the following components:

$$H_\zeta = \{0, \mathbf{p}_\Sigma, E_\Sigma, H_\Sigma, \mathbf{u}_\Sigma, \mathbf{F}_\Sigma\}, \quad (2.6)$$

where

$\mathbf{p}_\Sigma$ is the vector of surface stresses;

E_Σ is the energy of surface stresses;

H_Σ is the entropy release on the phase interface;

$\mathbf{u}_\Sigma$ is the incompatibility vector on the phase interface;

$\mathbf{F}_\Sigma$ is the incompatibility tensor on the phase interface.

The conditions (2.5) hold true on the phase interface Σ_{ij} for the case when phase transformations are absent. For this $D_0 = 0$, where D_0 is the *rate of phase transformation*, $D_0 = D - \mathbf{v}_i \cdot \mathbf{n}_i$.

2.2 Constitutive Relations for Phases of Ablative Composites

2.2.1 The Fourier Law

The conservation equation set (2.2) consists of $18n$ scalar equations for $29n$ functions, where n is the number of phases. To close the system one should complement it with

additional relations. One of them is the relationship connecting the heat flux vector $\mathbf{q}_i$ with the temperature gradient $\nabla\theta_i$ of phases:

$$\mathbf{q}_i = -\mathbf{k}_i \cdot \nabla\theta_i, \quad i = a, b, p, g, l, \quad (2.7)$$

and called *Fourier's law*.

The tensors $\mathbf{k}_i$ are the *heat conductivity tensors* of the phases.

2.2.2 General Thermodynamical Identity

The derivation of the remaining additional relations is based on thermodynamic equations (Eqs. (2.2) at $\zeta = 3$ and 4).

Let us introduce the *total derivative with respect to time* of an arbitrary function Ω_i defined within the domain V_i :

$$\frac{d_i \Omega_i}{dt} = \frac{\partial \Omega_i}{\partial t} + \mathbf{v}_i \cdot \nabla \Omega_i. \quad (2.8)$$

Let us also introduce *Almansi's finite strain tensor* $\mathbf{\Lambda}_i$ for solid phases $i = \{a, b, p, l\}$ connected to the strain gradient $\mathbf{F}_i$, the metric tensors components g^{ks} , $\overset{\circ}{g}^{ks}$ and the displacement vector $\mathbf{u}_i$ by the relationships

$$\begin{aligned} \mathbf{\Lambda}_i &= \frac{1}{2}(g^{ks} - \overset{\circ}{g}^{ks})\mathbf{r}_k \otimes \mathbf{r}_s = \frac{1}{2}(\mathbf{E} - \mathbf{F}_i^{-1} \cdot \mathbf{F}_i^{-T}) \\ &= \frac{1}{2}(\nabla \otimes \mathbf{u}_i + (\nabla \otimes \mathbf{u}_i)^T - (\nabla_x \otimes \mathbf{u}_i)^T \cdot \nabla \otimes \mathbf{u}_i). \end{aligned} \quad (2.9)$$

By taking account of Eq. (2.8), we can write the system (2.2) in the form

$$\rho_i \frac{d_i A_{i\zeta}}{dt} = \nabla B_{i\zeta} + C_{i\zeta}, \quad \zeta = 2, \dots, 5. \quad (2.10)$$

From the momentum equation (2.10) at $\zeta = 2$ we obtain the *equation of kinetic energy* for the phases

$$\rho_i \frac{d_i}{dt} \left(\frac{v_i^2}{2} \right) = \mathbf{v}_i \cdot \nabla \cdot \boldsymbol{\sigma}_i, \quad v_i^2 = \mathbf{v}_i \cdot \mathbf{v}_i. \quad (2.11)$$

The new function

$$\psi_i = e_i - \eta_i \theta_i \quad (2.12)$$

is called the *Helmholtz free energy* of the phase. From the energy equation (2.10) at $\zeta = 3$ and entropy balance at $\zeta = 4$, and Eq. (2.11), we derive the equation for ψ_i

$$\rho_i \frac{d_i \psi_i}{dt} + \rho_i \eta_i \frac{d_i \theta_i}{dt} - \boldsymbol{\sigma}_i \cdot \cdot \nabla \otimes \mathbf{v}_i + W_i^* = 0. \quad (2.13)$$

The stress tensor $\boldsymbol{\sigma}_i$ can be written in the form

$$\boldsymbol{\sigma}_i = \mathbf{T}_i + \mathbf{T}'_i, \quad (2.14)$$

where $\mathbf{T}_i$ is the tensor of *elastic stresses* and $\mathbf{T}'_i$ is the tensor of *viscous stresses*. The expression for power of elastic stresses of the i th phase $W_i = \mathbf{T}_i \cdot \cdot \nabla \otimes \mathbf{v}_i$ can be rewritten as follows by taking account of formulae (2.1) and (2.9) and the definition of total derivative (2.8):

$$W_i = \mathbf{T}_i \cdot \cdot \nabla \otimes \mathbf{v}_i = -\mathbf{T}_i \cdot \cdot \mathbf{F}_i \cdot \frac{d_i \mathbf{F}_i^{-1}}{dt} = \mathbf{F}_i^T \cdot \mathbf{T}_i \cdot \mathbf{F}_i \cdot \cdot \frac{d_i \boldsymbol{\Lambda}_i}{dt}. \quad (2.15)$$

On substituting Eqs. (2.14) and (2.15) into the formula (2.13), we obtain the so-called *general thermodynamical identity* for the i th phase

$$\rho_i \frac{d_i \psi_i}{dt} + \rho_i \eta_i \frac{d_i \theta_i}{dt} - \mathbf{F}_i^T \cdot \mathbf{T}_i \cdot \mathbf{F}_i \cdot \cdot \frac{d_i \boldsymbol{\Lambda}_i}{dt} - \mathbf{T}'_i \cdot \cdot \nabla \otimes \mathbf{v}_i + W_i^* = 0. \quad (2.16)$$

2.2.3 Natural Configurations of Phases

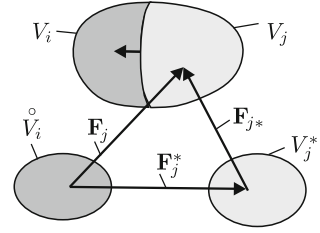
Further analysis is based on an additional assumption concerning the form of the functions ψ_i and tensors $\mathbf{T}'_i$ of viscous stresses for the phases. First we establish the general structure of the dependence of ψ_i on its arguments.

We assume that for each i th phase there exists a certain configuration V_i^* in which both stresses and strains are absent and the free energy ψ_i has a minimum. This configuration V_i^* is called *natural*. If in the composite the phase transformation ' $i \rightarrow j$ ' takes place, then for each phase, the natural configuration is assumed to be coincident with the initial one $\overset{\circ}{V}_i$. For the j th phase formed as a result of the phase transformation the configurations V_j^* and $\overset{\circ}{V}_j$ do not usually coincide. Moreover, since after the phase transformation in the j th phase a stress-strain state immediately appears, the natural configuration V_j^* can be unrealizable.

A scheme of the phase transformation ' $i \rightarrow j$ ' can be presented in the following way (Fig. 2.1). For the same point M with material coordinates X^k let the coordinates of the radius-vectors be $\overset{\circ}{\mathbf{x}}_i$, $\mathbf{x}_j$, $\mathbf{x}_j^*$, and infinitesimal elements of the radius-vectors $d\overset{\circ}{\mathbf{x}}_i$, $d\mathbf{x}_j$, $d\mathbf{x}_j^*$ in the configurations $\overset{\circ}{V}_i$, V_j and V_j^* , respectively. In each configuration we introduce the local basis vectors

$$\mathbf{r}_k = \partial \mathbf{x}_j / \partial X^k, \quad \overset{\circ}{\mathbf{r}}_k = \partial \overset{\circ}{\mathbf{x}}_i / \partial X^k, \quad \mathbf{r}_k^* = \partial \mathbf{x}_j^* / \partial X^k$$

Fig. 2.1 Schematic relation between natural and actual configurations of i th and j th phases



and components of metric tensors

$$g_{sk} = \mathbf{r}_s \cdot \mathbf{r}_k, \quad \overset{\circ}{g}_{sk} = \overset{\circ}{\mathbf{r}}_s \cdot \overset{\circ}{\mathbf{r}}_k, \quad g_{sk}^* = \mathbf{r}_s^* \cdot \mathbf{r}_k^*, \quad \mathbf{x}' \in V_j(t). \quad (2.17)$$

Transition of a local vicinity of the material point M of the i th phase from the initial configuration into the actual one is described by the strain gradient $\mathbf{F}_j$, and from V_j^* into V_j , by the strain gradient $\mathbf{F}_{j*}$:

$$d\mathbf{x}_j = \mathbf{F}_j \cdot d\overset{\circ}{\mathbf{x}}_i, \quad d\mathbf{x}_j = \mathbf{F}_{j*} \cdot d\mathbf{x}_j^*. \quad (2.18)$$

We introduce a strain gradient $\mathbf{F}_j^*$ called the *phase transformation gradient* which transforms a local vicinity of the material point M from the natural configuration $\overset{\circ}{V}_i$ of the i th phase into the natural configuration V_j^* of the j th phase:

$$d\mathbf{x}_j^* = \mathbf{F}_j^* \cdot d\overset{\circ}{\mathbf{x}}_i. \quad (2.19)$$

As follows from formulae (2.18) and (2.19), the transformation of the initial configuration $\overset{\circ}{V}_i$ into the actual one V_j can be presented by the superposition

$$\mathbf{F}_j = \mathbf{F}_{j*} \cdot \mathbf{F}_j^*. \quad (2.20)$$

Introduce components of the inverse metric tensors and vectors of coupling bases in the configuration V_j^*

$$g^{*ks} g_{sr}^* = \delta_r^k, \quad \mathbf{r}^{*k} = g^{*ks} \mathbf{r}_s^*. \quad (2.21)$$

Tensors $\mathbf{F}_{j*}$ and $\mathbf{F}_j^*$ are connected to the vectors of local bases by the relations

$$\mathbf{F}_{j*} = \mathbf{r}_k \otimes \mathbf{r}^{*k}, \quad \mathbf{F}_j^* = \mathbf{r}_k^* \otimes \overset{\circ}{\mathbf{r}}^k, \quad \mathbf{x}^k \in V_j. \quad (2.22)$$

Similarly to the formula (2.9), introduce Almansi's strain tensor $\mathbf{\Lambda}_{j*}$ describing a deformation of the j th phase at transition from the natural configuration V_j^* into the actual one V_j :

$$\Lambda_{j*} = \frac{1}{2}(g^{*sk} - g^{sk})\mathbf{r}_s^* \cdot \mathbf{r}_k^* = \frac{1}{2}(\mathbf{E} - \mathbf{F}_{j*}^{-1} \cdot \mathbf{F}_{j*}^{-T}). \quad (2.23)$$

On expressing the tensor $\mathbf{F}_{j*}$ from (2.20) and substituting this into (2.23), we obtain the relationship between strain tensors Λ_j and Λ_{j*} :

$$\Lambda_{j*} = \mathbf{F}_j^* \cdot \Lambda \cdot \mathbf{F}_j^{*T} + \frac{1}{2}(\mathbf{E} - \mathbf{F}_j^* \cdot \mathbf{F}_j^{*T}). \quad (2.24)$$

The phase transformation gradient $\mathbf{F}_j^*$ involved in the Eq.(2.24) is a ‘passport’ characteristic of the phase transformation $i \rightarrow j$ which should be given together with the model of the material. For the most actual problems the tensors $\mathbf{F}_j^*$ can be assumed to be constant and determined in independent specific experiments. Methods of definition of $\mathbf{F}_j^*$ will be given below. In fact, tensors $\mathbf{F}_j^*$ describe the appearance of shrinkage deformations at the phase transformations.

If the forming j th phase is gas ($j = g$), then one can also determine the natural configuration V_g^* of gas phase and the gradient of phase transformation $\mathbf{F}_g^*$ which has one independent component, being the density ρ_g^* :

$$\rho_g^* = \rho_g^0 \det(\mathbf{F}_g^{*-1}), \quad (2.25)$$

here $\det$ is the non-zero determinant of the tensor $(\mathbf{F}_g^*)^{-1}$.

2.2.4 General Form of Constitutive Relations

Let us consider the form of the free energy ψ_i of phases. The free energy ψ_i is assumed to be a functional of Almansi’s strain tensor Λ_{i*} and temperature θ_i with respect to time t :

$$\psi_i = \overset{t}{\underset{\tau=t_i^*}{\psi_i}} \left(\Lambda_{i*}(\tau) - \overset{\circ}{\Lambda}_i(\tau), \theta_i(\tau) \right), \quad i = a, b, p, l, g, \quad (2.26)$$

where $\overset{t}{\underset{\tau=t_i^*}{\psi_i}}$ means that the free energy ψ_i at time t depends on the prehistory of the tensor $\Lambda_{i*}(\tau)$ and temperature $\theta_i(\tau)$ during the time period $t_i^* \leq \tau \leq t$; here $t_i^*(\mathbf{x})$ is the time of origin of a material particle of the i th phase with coordinate $\mathbf{x}$.

The choice of tensor Λ_{i*} as an argument in Eq.(2.25) under the condition $\psi_i(\Lambda_{i*}, \theta_i) \geq \psi_i(0, \theta_0)$ ensures a minimum of the free energy in the natural configuration.

In the relationships (2.26) the following tensors are introduced

$$\overset{\circ}{\Lambda}_i = \alpha_i(\theta_i - \theta_i^*), \quad (2.27)$$

where α_i are the *tensors of heat expansion*, θ_j^* is the temperature of the j th phase in the actual configuration at time $t_j^*(\mathbf{x})$ of its appearance: $\theta_j^* = \theta_j(t_j^*(\mathbf{x}), \mathbf{x})$.

The total derivative (2.8) of ψ_i with respect to time is determined in accordance with the rule of differentiation of functionals [15, 16]:

$$\frac{d_i \psi}{dt} = \frac{\partial \psi_i}{\partial \Lambda_i} \cdot \frac{d_i \Lambda_i}{dt} + \frac{\partial \psi_i}{\partial \theta_i} \frac{d_i \theta_i}{dt} + \frac{\mathcal{D} \psi_i}{\mathcal{D} t}, \quad (2.28)$$

where $\mathcal{D} \psi_i / (\mathcal{D} t)$ is *Gateaux's derivative* [6, 15, 16], being a linear functional of pre-history of rates of change of the strain tensors $(d_i/d\tau)(\Lambda_{i*} - \overset{\circ}{\Lambda}_i)(\tau)$ and temperature $d_i \theta(\tau)/d\tau$.

On substituting the expression (2.28) into Eq.(2.16), from the condition that derivatives $(d_i \Lambda_i/dt)$ and $(d_i \theta_i/dt)$ are independent, we derive the general thermodynamic identity (2.16) which is equivalent to the simultaneous relations

$$\mathbf{T}_i = \rho_i \mathbf{F}_i^{-T} \cdot \mathbf{F}_i^{*T} \cdot \frac{\partial \psi_i}{\partial \Lambda_{i*}} \cdot \mathbf{F}_i^* \cdot \mathbf{F}_i^{-1}, \quad (2.29)$$

$$W_i^* = \mathbf{T}_i' : \nabla \otimes \mathbf{v}_i - \rho_i \frac{\mathcal{D} \psi_i}{\mathcal{D} t}, \quad (2.30)$$

$$\eta_i = -\partial \psi_i / \partial \theta_i. \quad (2.31)$$

called *constitutive relations for phases* of the composite.

The expression (2.12) for the internal energy of the i th phase e_i , on taking (2.31) into account, has the form

$$e_i = \psi_i - \theta_i \frac{\partial \psi_i}{\partial \theta_i}. \quad (2.32)$$

Formulae (2.23) and (2.24) connect tensors Λ_{i*} to Λ_i and $\mathbf{F}_i^*$ and hence to $\mathbf{F}_i^{-1}$ and $\mathbf{F}_i^*$; thus $\mathbf{T}_i$ in Eq. (2.29) depends on $\mathbf{F}_i^{-1}$ and $\mathbf{F}_i^*$.

In order to establish a specific form of the relations (2.29)–(2.31), one should define the following:

- the specific dependence (2.26) for the free energies ψ_i ;
- the values of the phase transformation gradients $\mathbf{F}_i^*$;
- the specific expression for the viscous stress tensor depending on the velocity gradient: $\mathbf{T}_i' (\nabla \otimes \mathbf{v}_i)$.

Below, for solid phases of the composite it is assumed that $\mathbf{T}_i' = 0$.

When there are no phase transformations,

$$\mathbf{F}_i^* = \mathbf{E}, \quad \Lambda_i^* = \Lambda_i, \quad \Lambda_{i*} = 0, \quad t_i^* = 0, \quad \theta_i^* = \theta_0, \quad (2.33)$$

and constitutive relations (2.29), with account (2.26), are transformed as follows:

$$\mathbf{T}_i = \rho_i \mathbf{F}_i^{-T} \cdot \frac{\partial \psi}{\partial \mathbf{\Lambda}_i} \cdot \mathbf{F}_i^{-1}; \quad (2.34)$$

here $\mathbf{T}_i$ depend only on $\mathbf{\Lambda}_i$ and θ_i .

Gas phase ($i = g$) of the composite is assumed to be *linear-viscous*, i.e. ψ_g and $\mathbf{T}'_g$ have the form

$$\psi_g = \psi_g(\rho_g, \rho_g^*, \theta_g), \quad (2.35)$$

$$\mathbf{T}'_g = \nu_g \mathbf{E} \nabla \cdot \mathbf{v}_g + \mu_g (\nabla \otimes \mathbf{v}_g + (\nabla \otimes \mathbf{v}_g)^T), \quad (2.36)$$

where ν_g, μ_g are the viscosity coefficients. The phase transformation gradient $\mathbf{F}_g^*$ for the gas phase has one independent component, the gas phase density ρ_g^* in its natural configuration introduced by formula (2.25).

Then constitutive relations (2.29)–(2.31) for the gas phase take the form

$$\mathbf{T}_g = -p \mathbf{E}, \quad p = \rho_g^2 \frac{\partial \psi_g}{\partial \rho_g}, \quad \eta_g = -\frac{\partial \psi_g}{\partial \theta_g}, \quad W_g^* = \mathbf{T}'_g \cdot \cdot \nabla \otimes \mathbf{v}_g. \quad (2.37)$$

Here it is taken into consideration that [16, 29]

$$\partial \rho / \partial \mathbf{\Lambda} = -\rho \mathbf{F}^T \cdot \mathbf{F}, \quad (2.38)$$

and pressure of the gas phase is denoted by p .

Thus, constitutive relations for phases of the composite are defined completely by formulae (2.7), (2.29)–(2.32) and (2.35)–(2.37) connecting functions $\mathbf{q}_i, W_i^*, \eta_i, e_i, \boldsymbol{\sigma}_i$ to $\rho_i, \mathbf{v}_i, \mathbf{u}_i, \theta_i$. Herein it is taken into account that strain gradients $\mathbf{F}_i^{-1}$ and strain tensors $\mathbf{\Lambda}_i$ are expressed in terms of displacement vectors $\mathbf{u}_i$ of phases by formulae (2.1) and (2.9).

On substituting the constitutive relations (2.7), (2.29)–(2.32) and (2.35)–(2.37) into Eqs. (2.2), we obtain the closed system of $8n$ scalar equations at $\zeta = 1, 2, 3, 5$ (equation at $\zeta = 4$ for entropy balance is excluded; the assumptions (2.26) and (2.35) for free energies of the phases make it equivalent to the constitutive relations) for $8n$ functions: $\rho_i, \mathbf{v}_i, \mathbf{u}_i, \theta_i$ ($i = a, b, p, g, l$), where $n = 5$ is the number of phases.

It should be noted that, for the gas phase, the kinematic equations (2.2) at $\zeta = 5$ for the displacement vector $\mathbf{u}_i$ can not be considered, thus, the number of equations and unknown functions in the set decreases by $3n_g$, where n_g is the number of gas phases in the multiphase medium (for the considered ablative composite $n_g = 1$).

2.3 Relations at the Phase Interface

2.3.1 Main Equations

Relations (2.5) at the phase interface Σ_{ij} between the i th and j th phases can be written in the explicit form

$$[\rho(D - \mathbf{v} \cdot \mathbf{n})] = 0, \quad (2.39)$$

$$\mathbf{M}[\mathbf{v}] + \mathbf{n} \cdot [\boldsymbol{\sigma}] = \mathbf{p}_\Sigma, \quad (2.40)$$

$$\mathbf{M}[e + \frac{v^2}{2}] + \mathbf{n} \cdot [\boldsymbol{\sigma} \cdot \mathbf{v} - \mathbf{q}] = E_\Sigma, \quad (2.41)$$

$$\mathbf{M}[\eta] - \mathbf{n} \cdot [\mathbf{q}/\theta] = H_\Sigma, \quad (2.42)$$

$$\mathbf{M}[\mathbf{u}] = \mathbf{u}_\Sigma, \quad (2.43)$$

$$\mathbf{M}[\mathbf{F}] + [\rho \mathbf{v} \otimes \mathbf{F}^T] \cdot \mathbf{n} = \mathbf{F}_\Sigma, \quad \mathbf{x} \in \Sigma_{ij}, \quad (2.44)$$

where $\mathbf{M}$ is the *mass rate of the phase transformation* connected to the rate D_0 by the relationship

$$\mathbf{M} = \rho_i(D - \mathbf{v}_i \cdot \mathbf{n}) = \rho_i D_0. \quad (2.45)$$

As the i th phase, for which the phase transformation rate D_0 is considered, a solid phase is usually chosen for phase transformation of the type ‘solid phase $\rightleftharpoons$ gas’, and the ‘old’ solid phase is used for the phase transformation ‘old solid phase $\rightleftharpoons$ new solid phase’.

In addition, at the phase interface Σ_{ij} the following condition of continuity of the radius-vector is always satisfied:

$$[\mathbf{x}] = 0,$$

this means that there is no delamination between the phases.

The appearance of the functions $\mathbf{p}_\Sigma$, E_Σ in (2.40) and (2.41) determined on the phase interface is usually connected to the phenomenon of surface tension. In this case

$$\mathbf{p}_\Sigma = P_\Sigma \mathbf{n}, \quad P_\Sigma = -\sigma_\Sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right), \quad (2.46)$$

where σ_Σ is the surface tension coefficient on the phase interface, and R_1 , R_2 are the principal radii of curvature of the phase interface Σ_{ij} at the given point $\mathbf{x} \in \Sigma_{ij}$.

The surface tension energy E_Σ is determined by the formula

$$E_\Sigma = \mathbf{p}_\Sigma \cdot \{\mathbf{v}\}, \quad (2.47)$$

where $\{\Omega\}$ is the mean value of functions Ω_i and Ω_j at the phase interface:

$$\{\Omega\} = \frac{1}{2} (\Omega_i|_{\mathbf{x} \in \Sigma_{ij}} + \Omega_j|_{\mathbf{x} \in \Sigma_{ij}}). \quad (2.48)$$

Entropy production H_Σ at the phase transformation surface is always nonnegative $H_\Sigma \geq 0$.

We introduce a gradient of strain incompatibility $\mathbf{F}'_\Sigma$ and a vector of discontinuity displacement $\mathbf{u}'_\Sigma$ connected to $\mathbf{F}_\Sigma$ by the relationships

$$\mathbf{F}_\Sigma = (\mathbf{M}\mathbf{E} + \rho_j \mathbf{v}_j \otimes \mathbf{n}) \cdot \mathbf{F}'_\Sigma, \quad \mathbf{u}_\Sigma = \mathbf{M}\mathbf{u}'_\Sigma. \quad (2.49)$$

2.3.2 Classification of Phase Interfaces

The form of the surface functions H_Σ and $\mathbf{u}'_\Sigma$ does not generally follow from the general equations of thermomechanics, but is defined by the type of the phase interface.

A phase interface Σ_{ij} is called *nondissipative* if the following condition is satisfied:

$$H_\Sigma = 0, \quad \mathbf{x} \in \Sigma_{ij}. \quad (2.50)$$

If the conditions

$$\mathbf{u}'_\Sigma = 0, \quad \mathbf{F}'_\Sigma = 0, \quad \mathbf{x} \in \Sigma_{ij}, \quad (2.51)$$

are satisfied, then Σ_{ij} is called the phase interface *with ideal contact*. At this surface two arbitrary neighboring material points on different sides of the surface remain neighboring for all deformations, and only the strain state in the vicinity of the points changes.

A phase interface *with slip* is a surface Σ_{ij} for which the following conditions are satisfied:

$$\mathbf{u}'_\Sigma = -[\dot{\mathbf{x}}] \neq 0, \quad \mathbf{F}'_\Sigma \neq 0, \quad \mathbf{x} \in \Sigma_{ij}. \quad (2.52)$$

For a phase interface with slip, neighboring points on different sides of the surface at time t_1 can displace by time t_2 along the surface Σ_{ij} without leaving the surface, i.e. delaminations between the phases are not permitted.

Surface Σ_{ij} is called a *surface of phase transformation* if

$$D_0 \neq 0.$$

Phase transformations with ideal contact at the surface are characteristic for transitions of the type: solid phase $\rightarrow$ new solid phase, and also solid phase $\rightarrow$ viscous gas (liquid).

Phase transformations with slip on their surfaces are, in particular, transitions: solid phase $\rightarrow$ ideal gas (liquid). For surfaces with slip there appear additional unknown values, namely vector $\mathbf{u}'_{\Sigma}$ and tensor $\mathbf{F}'_{\Sigma}$. For case of the phase transformation: solid phase $\rightarrow$ ideal gas values of $\mathbf{F}'_{\Sigma}$ and $\mathbf{u}'_{\Sigma}$ are determined from the relations (2.43) and (2.44), which are not involved in the problem statement for the determination of the main functions $\rho_i, \rho_j, \mathbf{v}_i, \mathbf{v}_j, \theta_i, \theta_j$ and $\mathbf{u}_i$ for the set (2.2).

A phase interface Σ_{ij} is called *homothermal*, if there is no temperature jump on the surface:

$$[\theta] = 0, \quad \mathbf{x} \in \Sigma_{ij}. \quad (2.53)$$

For most practical problems of phase transformations, including the problems for ablative composites, assumptions (2.50) and (2.53) on homothermicity and nondissipativity are justified, and allow us to describe adequately enough the actual processes of phase transformations.

2.3.3 Consequences of General Equations

Let us show several important consequences of relations (2.39)–(2.44) for a phase interface, which is assumed to be homothermal, nondissipative and with slip.

The scalar product of Eq.(2.40) and vector $\{\mathbf{v}\}$ is the analog of the equation of kinetic energy (2.11) for the phase interface:

$$M[v^2/2] + \mathbf{n} \cdot [\boldsymbol{\sigma}] \cdot \{\mathbf{v}\} = \mathbf{p}_{\Sigma} \cdot \{\mathbf{v}\}. \quad (2.54)$$

From Eqs.(2.41), (2.42), (2.50) and (2.53) we can derive the expression for the jump of the Helmholtz free energy ψ_i determined by formula (2.12)

$$M[\psi] + \mathbf{n} \cdot \{\boldsymbol{\sigma}\} \cdot [\mathbf{v}] = E_{\Sigma} - \mathbf{p}_{\Sigma} \cdot \{\mathbf{v}\}. \quad (2.55)$$

We introduce new tensors $\mathbf{F}'_i$ and $\mathbf{F}'_j$ connected to $\mathbf{F}_i$ and $\mathbf{F}_j$ by the relations

$$\mathbf{F}'_i = \mathbf{F}_i, \quad \mathbf{F}'_j = \mathbf{F}_j + \mathbf{F}'_{\Sigma}. \quad (2.56)$$

It is evident that $[\mathbf{F}'] = [\mathbf{F}] - \mathbf{F}'_{\Sigma}$.

Having multiplied scalarly Eq.(2.44) by normal vector $\mathbf{n}$ and substituted Eqs.(2.45) and (2.39) into the product, we obtain the expression for the jump of the phase strain gradient

$$[\rho \mathbf{F}'^T] \cdot \mathbf{n} = 0. \quad (2.57)$$

On multiplying Eq.(2.44) on the right side by $\mathbf{F}_i^{-1} \cdot \mathbf{n}$ and using formula (2.57), we derive the expression for the jump of phase velocities through the phase interface

$$[\mathbf{v}] = -\frac{M}{\rho_i} [\mathbf{F}'] \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n}. \quad (2.58)$$

If relation (2.44) is multiplied on the left side by vector $\mathbf{F}_j'^{-1} \cdot \mathbf{n}$, then the formula (2.58) also follows, with index j replaced by i . On comparing this formula with Eq. (2.58), we find the relationship inverse to (2.57)

$$[\mathbf{F}'^{-1}/\rho] \cdot \mathbf{n} = 0. \quad (2.59)$$

On substituting Eq. (2.58) into formula (2.40), we obtain the expression for the jump of normal stress in the phases

$$\mathbf{n} \cdot [\boldsymbol{\sigma}] = \frac{M^2}{\rho_i} [\mathbf{F}'] \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n} + \mathbf{p}_\Sigma. \quad (2.60)$$

Then having substituted the expression for the velocity jump (2.58) and Eq. (2.47) for E_Σ into Eq. (2.55) and performed algebraic transformations of the type

$$\mathbf{n} \cdot \{\boldsymbol{\sigma}\} \cdot [\mathbf{F}'] \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n} = \mathbf{n} \cdot [\boldsymbol{\sigma} \cdot \mathbf{F}'] \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n} - \mathbf{n} \cdot [\boldsymbol{\sigma}] \cdot \{\mathbf{F}'\} \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n},$$

we rewrite the relation (2.55) as follows:

$$[\psi] - \frac{1}{\rho_i} \mathbf{n} \cdot [\boldsymbol{\sigma} \cdot \mathbf{F}'] \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n} + \frac{1}{\rho_i} \mathbf{n} \cdot [\boldsymbol{\sigma}] \cdot \{\mathbf{F}'\} \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n} = 0. \quad (2.61)$$

On substituting Eq. (2.60) into relation (2.61) and taking the property (2.59) of tensor $\mathbf{F}_i'^{-1}/\rho$ into account, we find

$$[\psi] - \mathbf{n} \cdot [\boldsymbol{\sigma}/\rho] \cdot \mathbf{n} + \frac{M^2}{2\rho_i} \mathbf{n} \cdot \mathbf{F}_i^{\text{T}-1} \cdot [\mathbf{F}^{\text{T}'} \cdot \mathbf{F}'] \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n} + 2P_\Sigma\{1/\rho\} = 0. \quad (2.62)$$

2.3.4 Tensor of Chemical Potential

We introduce two new second-order tensors for each α th phase $\alpha \in \{i, j\}$, where $i, j \in \{a, b, p, g, l\}$, namely the symmetric tensor χ_α called the *Bowen's tensor of chemical potential*, and the symmetric one $\mathbf{K}_\alpha$ called the *tensor of kinetic energy of phase transformation*:

$$\chi_\alpha = \psi_\alpha \mathbf{E} - \frac{\boldsymbol{\sigma}_\alpha}{\rho_\alpha}, \quad \mathbf{K}_\alpha = \frac{M^2}{2\rho_i} \mathbf{F}_i^{\text{T}-1} \cdot \mathbf{F}_\alpha^{\text{T}'} \cdot \mathbf{F}_\alpha' \cdot \mathbf{F}_i^{-1}, \quad (2.63)$$

$$\alpha \in \{i, j\}, \quad i, j \in \{a, b, p, g, l\}.$$

Then the relation (2.62) takes the final form

$$\mathbf{n} \cdot [\chi + \mathbf{K}] \cdot \mathbf{n} + 2P_\Sigma\{1/\rho\} = 0. \quad (2.64)$$

Tensors χ_α as well as internal energy, free energy etc. are thermodynamical characteristics of phases; they are independent of a phase geometry in explicit form and depend only on phase characteristics θ_i , $\mathbf{F}_i$, ρ_i etc.

The expression (2.63) for $\mathbf{K}_\alpha$ has been written for phase transformations with slip on their surface. For phase transformations without slip the relation (2.64) holds, but the expression for $\mathbf{K}_\alpha$ can be written in a simpler form

$$\mathbf{K}_\alpha = \frac{M^2}{2\rho_i} \mathbf{F}_i^{\text{T}-1} \cdot \mathbf{F}_\alpha^{\text{T}} \cdot \mathbf{F}_\alpha \cdot \mathbf{F}_i^{-1}, \quad (2.63a)$$

as for χ_α , this expression is independent of a phase geometry.

Relation (2.60) for surfaces without slip can be simplified as well

$$\mathbf{n} \cdot [\sigma] = \frac{M^2}{\rho_i} [\mathbf{F}] \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n} + \mathbf{p}_\Sigma. \quad (2.60a)$$

2.4 Equation of Phase Transformation Rate

The phase transformation rate D_0 introduced in formula (2.4) as the rate of motion of the phase interface Σ_{ij} (in particular, of phases $i = b$ and $j = p$, and also $i = b$ and $j = g$) characterizes the rate of volumetric ablation of composite material according to the classification given in Sect. 1.2. This rate D_0 is not constant and depends on the temperature θ_i of the phases on their interface and, generally speaking, on stresses σ_i and σ_j , densities ρ_i , ρ_j and possibly on other characteristics of the phases. This dependence

$$D_0 = D_0(\theta_i, \theta_j, \sigma_i, \sigma_j, \rho_i, \rho_j), \quad \mathbf{x} \in \Sigma_{ij} \quad (2.65)$$

as well as constitutive relations for phases (2.29)–(2.31), characterizes physical properties of the phase substance. The constitutive relations obey certain thermodynamical restrictions which are a consequence of the equation of entropy balance ($\zeta = 4$) from the set (2.2) and have a certain structure (2.29)–(2.31).

The phase transformation rate also satisfies some restrictions and cannot be given in an arbitrary way. These restrictions are a consequence of the Eq. (2.5) at $\zeta = 4$ for entropy balance on the phase interface.

As shown in Sect. 2.3, the relation (2.64) for chemical potential is a consequence of the equation of entropy balance (2.5) at $\zeta = 4$. We use the relation to derive an expression for the rate D_0 .

Let us consider a phase interface without slip.

If the constitutive relations of phases (2.29)–(2.31) have been substituted into Eqs. (2.64) for tensors χ_α and $\mathbf{K}_\alpha$, where functions $\psi_i, \psi_j, \mathbf{F}_i, \mathbf{F}_j$ have been expressed in terms of stresses σ_i, σ_j , temperature θ_i and density ρ_i, ρ_j of phases (one should invert the relations (2.29) and express $\mathbf{A}_i$ in terms of σ_i and then substitute them into (2.26)), and, in addition, M^2 has been expressed from Eq. (2.60a) and substituted into (2.63), then the relation (2.64) takes the form of an equation connecting the functions $\sigma_i, \sigma_j, \rho_i, \rho_j$ and θ_i of the phases

$$\Phi_n(\sigma_i, \sigma_j, \rho_i, \rho_j, \theta_i) = 0, \quad \mathbf{x} \in \Sigma_{ij}. \quad (2.66)$$

Subscript n indicates that the equation depends on the geometry of the phase transformation surface.

The Eq. (2.66) can be used to express the normal stress of the j th phase on the phase interface $\sigma_{nj} = -\mathbf{n} \cdot \sigma_j \cdot \mathbf{n}$ in terms of all the remaining arguments $\sigma_i, \rho_i, \rho_j, \theta$, and also of tangential stresses τ_j on the phase interface determined as $\tau_j = \sigma_j - \sigma_{nj} \mathbf{n} \otimes \mathbf{n}$:

$$\sigma_{nj} = S_n(\sigma_i, \tau_j, \rho_i, \rho_j, \theta), \quad \mathbf{x} \in \Sigma_{ij}. \quad (2.67)$$

In a similar way we determine σ_{ni} for the i th phase: $\sigma_{ni} = -\mathbf{n} \cdot \sigma_i \cdot \mathbf{n}$. Having multiplied the Eq. (2.60) scalarly by vector $\mathbf{n}$ and solved the obtained equation for M^2 , and taken Eq. (2.67) into account, we get

$$M^2 = \frac{\rho_i(S_n - \sigma_{ni} - P_\Sigma)}{\mathbf{n} \cdot [\mathbf{F}] \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n}}. \quad (2.68)$$

This equation is the desired expression for the mass rate of the phase transformation. From this equation and Eq. (2.45) we can derive an equation of the type (2.65) for the linear rate of the phase transformation:

$$D_0 = \left(\frac{S_n - \sigma_{ni} - P_\Sigma}{\rho_i \mathbf{n} \cdot [\mathbf{F}] \cdot \mathbf{F}_i^{-1} \cdot \mathbf{n}} \right)^{1/2}. \quad (2.68a)$$

It should be noted, that the expression (2.68a) (or (2.68)) for phase transformation is not identical to the relation (2.40) (or (2.60)), as the normal stress σ_{nj} is replaced by the expression (2.67) obtained, in its turn, from the condition (2.42) for entropy balance on the phase interface. In fact, the Eqs. (2.40) and (2.68a) are two different relations, the first of which is used for determination of a jump of normal stress of the phases, and the second is applied to define the phase transformation rate.

A specific expression for the function S_n and rate D_0 of phase transformations in ablative composite materials will be given below.

We now establish a connection between the location of the phase interface Σ_{ij} in the actual configuration, and the rate D_0 . Let the shape of the smooth phase interface

Σ_{ij} in the actual configuration be described by the equation

$$f_{ij}(\mathbf{x}, t) = 0. \quad (2.69)$$

On evaluating the total differential df_{ij} of the function, we obtain

$$df_{ij} = \frac{\partial f_{ij}}{\partial t} + D\mathbf{n} \cdot \nabla f_{ij} = 0.$$

If we use the definition of the normal vector $\mathbf{n}$ as a normalized gradient to the surface:

$$\mathbf{n} = \frac{\nabla f_{ij}}{|\nabla f_{ij}|}, \quad |\nabla f_{ij}| = (\nabla f_{ij} \cdot \nabla f_{ij})^{1/2}, \quad (2.70)$$

and instead of the rate D its expression from (2.45), then we finally obtain

$$\frac{\partial f_{ij}}{\partial t} + \mathbf{v}_i \cdot \nabla f_{ij} + D_0 |\nabla f_{ij}| = 0, \quad t > t_i^*. \quad (2.71)$$

This differential equation with the initial condition

$$t = t_j^*, \quad f_{ij} = f_{ij}^0(\mathbf{x}) \quad (2.71a)$$

completely defines the location of the interface Σ_{ij} between the i th and j th phases in the actual configuration, if the phase transformation rate D_0 is known. Herein $f_{ij}^0(\mathbf{x})$ is the equation of the phase interface at the time of origin of the j th phase.

2.5 Infinitesimal Strains of Solid Phases

2.5.1 Main Assumptions

Most composite materials are stiff, i.e. their maximum ultimate deformations do not exceed 1–3 %. For such materials an additional assumption on *infinitesimal strains* is admissible, which can be formulated as follows: typical values of the strain gradients $\mathbf{F}_i$ for all solid phases and also phase transformation gradients $\mathbf{F}_i^*$ are close to unity:

$$\begin{aligned} \Delta \mathbf{F}_i &= \mathbf{E} - \mathbf{F}_i, \quad \|\Delta \mathbf{F}_i\| \ll 1, \quad i = a, b, p, l, \\ \beta_i &= \mathbf{E} - \mathbf{F}_i^*, \quad \|\beta_i\| \ll 1, \end{aligned} \quad (2.72)$$

where $\|\Delta \mathbf{F}_i\|$ is the typical value of components of tensor $\Delta \mathbf{F}_i$.

From Eqs. (2.72) we deduce the following:

- (a) in all equations of the general system (2.2) for the solid phases convective terms $\nabla \cdot \rho_i \mathbf{v}_i A_{ik}$ can be neglected as compared with the terms $\partial \rho_i A_{ik} / \partial t$ and $\nabla \cdot B_{ik}$; the form of the equations will be given below;
- (b) initial $\overset{\circ}{V}_i$ and actual V_i configurations for all solid phases are indistinguishable;
- (c) strain tensors $\mathbf{A}_i$ of phases depend linearly on the displacement gradients $\nabla \otimes \mathbf{u}_i$:

$$\mathbf{A}_i = \boldsymbol{\varepsilon}_i \equiv \frac{1}{2} (\nabla \otimes \mathbf{u}_i + (\nabla \otimes \mathbf{u}_i)^T), \quad (2.73)$$

- (d) strain tensors $\mathbf{A}_{i*}$ of phases depend linearly on $\nabla \otimes \mathbf{u}_i$ and $\boldsymbol{\beta}_i$:

$$\mathbf{A}_{i*} = \boldsymbol{\varepsilon}_i + \boldsymbol{\beta}_i. \quad (2.74)$$

The tensors $\boldsymbol{\beta}_j$ are called the *tensors of chemical shrinkage*, they characterize the deformation of the vicinity of the material point due to its phase transformation (when there is no mechanical load). For most ablative composites this deformation leads to a decrease in the volume of the material (shrinkage), which can be determined in experiments. The components of tensor $\boldsymbol{\beta}_j$ are evaluated by experimental values of composite shrinkage. This problem will be considered in detail below. When phase transformations are absent

$$\boldsymbol{\beta}_i = 0, \quad (2.75)$$

- (e) strain gradients $\mathbf{F}_i$ of solid phases can be assumed to be coincident with the unit tensor:

$$\mathbf{F}_i = \mathbf{E}. \quad (2.76)$$

2.5.2 Constitutive Relations

Solid Phases

Equations (2.26) and (2.29) show that for the case of infinitesimal strains the free energy ψ_i and stress tensor $\boldsymbol{\sigma}_i$ of solid phases depend on $\boldsymbol{\varepsilon}_i$ and θ_i .

The general thermodynamical identity (2.16) takes the form

$$\rho_i \frac{d\psi_i}{dt} - \boldsymbol{\sigma}_i \cdot \frac{d\boldsymbol{\varepsilon}_i}{dt} + \rho_i \eta_i \frac{d\theta_i}{dt} + W_i^* = 0, \quad \mathbf{x} \in V_i, \quad (2.77)$$

and the expression (2.26) for free energy ψ_i is rewritten as:

$$\psi_i = \psi_i^0 + \psi_i^\theta(\theta_i) + \psi_i^\varepsilon(\boldsymbol{\varepsilon}_i - \overset{\circ}{\boldsymbol{\varepsilon}}_i, \theta_i), \quad (2.78)$$

$\tau=0$

where ψ_i^θ depends only on current temperature $\theta_i(t)$ and ψ_i^ε —only on the prehistory of changing temperature $\theta_i(\tau)$, $0 \leq \tau < t$ and strains $(\varepsilon_i - \overset{\circ}{\varepsilon}_i)(\tau)$, $0 \leq \tau \leq t$. The tensor $\overset{\circ}{\varepsilon}_i = \overset{\circ}{\mathbf{A}}_i - \beta_i$, introduced in Eq. (2.78), is called the *tensor of heat deformations* and in accordance with formula (2.27) can be written in the form

$$\overset{\circ}{\varepsilon}_i = \alpha_i(\theta_i - \theta_i^*) - \beta_i, \quad (2.79)$$

The constitutive relations (2.29)–(2.31) for the case of infinitesimal strains take the form

$$\begin{aligned} \sigma_i &= \mathcal{F}_i(\varepsilon_i, \theta_i) = \rho_i \frac{\partial \psi_i}{\partial \varepsilon_i}, \\ \eta_i &= -\frac{\partial \psi_i}{\partial \theta_i}, \quad W_i^* = -\rho_i \frac{\mathcal{D} \psi_i}{\mathcal{D} t}. \end{aligned} \quad (2.80)$$

If solid phases are *linear-elastic* media, then the free energy ψ_i is a quadratic function of ε_i [16]:

$$\begin{aligned} \psi_i &= \psi_i^0 + \psi_i^\theta + \psi_i^\varepsilon, \\ \psi_i^\theta &= \int_{\theta_0}^{\theta_i} c_i d\theta_i - \theta_i \int_{\theta_0}^{\theta_i} \frac{c_i}{\theta_i} d\theta_i, \quad \psi_i^0 = e_i^0 - \theta_i \eta_i^0, \\ \psi_i^\varepsilon &= \frac{1}{2\rho_i} (\varepsilon_i - \overset{\circ}{\varepsilon}_i) \cdot \cdot \mathbf{C}_i \cdot \cdot (\varepsilon_i - \overset{\circ}{\varepsilon}_i), \end{aligned} \quad (2.81)$$

where c_i are the *heat capacities of the phases*.

The expression (2.32) for the internal energy e_i of phases is now written as follows:

$$e_i = e_i^0 + \int_{\theta_0}^{\theta_i} c_i d\theta_i + \psi_i^{\varepsilon} + \frac{1}{\rho_i} \alpha_i \cdot \cdot \sigma_i \theta_i, \quad (2.82)$$

and the constitutive relations (2.80) take the simple form

$$\sigma_i = \mathbf{C}_i \cdot \cdot (\varepsilon_i - \overset{\circ}{\varepsilon}_i), \quad W_i^* = 0, \quad (2.83)$$

$$\eta_i = \eta_i^0 + \int_{\theta_0}^{\theta_i} \frac{c_i}{\theta_i} d\theta_i + \frac{1}{\rho_i} \alpha_i \cdot \cdot \sigma_i,$$

where $e_i^0, \eta_i^0 = \text{const}$ are the initial values of internal energy and entropy of the i th phase.

The tensor $\mathbf{C}_i$ is called the *tensor of elastic moduli* of the solid phases.

Relations inverse to Eqs. (2.83) have the form

$$\varepsilon_i = \overset{\circ}{\varepsilon}_i + \mathbf{\Pi}_i \cdot \cdot \boldsymbol{\sigma}_i, \quad (2.84)$$

where the tensor $\mathbf{\Pi}_i$, called the *tensor of elastic pliabilities*, is inverse to $\mathbf{C}_i$: $\mathbf{C}_i \cdot \cdot \mathbf{\Pi}_i = \mathbf{\Delta}$, here $\mathbf{\Delta}$ is the unit fourth-order tensor [16].

As a rule, phases of composite material can be considered as *isotropic* media. In this case, Eqs. (2.83) and Fourier's law (2.7) can be simplified:

$$\boldsymbol{\sigma}_i = \left(\lambda_i \varepsilon_i - (3\lambda_i + 2\mu_i) \overset{\circ}{\varepsilon}_i \right) \mathbf{E} + 2\mu_i \varepsilon_i, \quad (2.85)$$

$$\mathbf{q}_i = -k_i \nabla \theta_i, \quad i = a, b, p, l, \quad (2.86)$$

where λ_i, μ_i are *Lamé's coefficients* of the i th phase, k_i is the heat conductivity coefficient of the i th phase and $\overset{\circ}{\varepsilon}_i$ is the heat deformation:

$$\overset{\circ}{\varepsilon}_i = \alpha_i (\theta - \theta_i^*) - \beta_i, \quad i = a, b, p, l, \quad (2.87)$$

$$\beta_a = \beta_b = \beta_l = 0, \quad \beta_p \neq 0.$$

Here α_i is the *heat expansion coefficient*, β_i is the *chemical shrinkage coefficient* of the i th phase. The Eq. (2.84) for an isotropic medium has the form

$$\varepsilon_i = \overset{\circ}{\varepsilon}_i \mathbf{E} + \frac{1 + \nu_i}{E_i} \boldsymbol{\sigma}_i - \frac{\nu_i}{E_i} \sigma_i \mathbf{E}, \quad (2.84a)$$

where $\sigma_i = \boldsymbol{\sigma}_i \cdot \cdot \mathbf{E}$, $\varepsilon_i = \varepsilon_i \cdot \cdot \mathbf{E}$ are the *first invariants* of tensors $\boldsymbol{\sigma}_i$ and ε_i , ν_i and E_i are the *Poisson's ratios* and elastic moduli connected to λ_i and μ_i by the relations

$$\mu_i = \frac{E_i}{2(1 + \nu_i)}, \quad \lambda_i = \frac{\nu_i E_i}{(1 + \nu_i)(1 - 2\nu_i)}.$$

Gas Phase

Gas phase is assumed below to be *perfect*, linear-viscous gas. Then the expression for free energy of the gas phase ψ_g (2.35) takes the form [16]

$$\psi_g = \psi_g^0 + \int_{\theta_0}^{\theta_g} c_g d\theta_g - \theta_g \int_{\theta_0}^{\theta_g} \frac{c_g}{\theta_g} d\theta_g - R\theta_g \ln(\rho_g^*/\rho_g), \quad (2.88)$$

where $\psi_g^0 = e_g^0 - \eta_g^0 \theta_g$, and the relations (2.37) are written as follows:

$$\begin{aligned}
\boldsymbol{\sigma}_g &= -p\mathbf{E} + \mathbf{T}'_g, \\
p &= R\rho_g\theta_g, \\
\mathbf{T}'_g &= \nu_g\mathbf{E}\nabla \cdot \mathbf{v}_g + \mu_g(\nabla \otimes \mathbf{v}_g + (\nabla \otimes \mathbf{v}_g)^\top), \\
e_g &= e_g^0 + \int_{\theta_0}^{\theta_g} c_g d\theta_g, \quad \eta_g = \eta_g^0 + \int_{\theta_0}^{\theta_g} \frac{\bar{c}_g}{\theta_g} d\theta_g - R \ln(p/p^*). \quad (2.89)
\end{aligned}$$

Here R is the *gas constant*, c_g is the heat capacity of the gas phase at constant volume, $\bar{c}_g = R + c_g$ is the heat capacity at constant pressure and ρ_g^* , $p^* = \rho_g^* R \theta_0$ are the density and pressure of the gas phase in the natural configuration under temperature θ_0 .

2.5.3 Quasistatic Processes

For current heat-loaded structures the most widespread case of high-temperature actions is the case of *quasistatic processes* of heating (see Chap. 1). The assumption on quasistaticity means that all processes in the composite propagate relatively slowly in time without dynamical (inertia) phenomena. Therefore:

- in the momentum equations (2.2) at $\zeta = 2$ for all n phases the inertial terms $\partial \rho_i \mathbf{v}_i / \partial t$ and $\nabla \rho_i \mathbf{v}_i \otimes \mathbf{v}_i$ can be neglected when compared with $\nabla \cdot \boldsymbol{\sigma}_i$;
- in the energy equations (2.2) at $\zeta = 3$ for all phases the kinetic energy of phase motion $\rho_i v_i^2 / 2$ can be neglected when compared with internal energy of phases $\rho_i e_i$;
- in the equations on the phase interface (2.5) at $\zeta = 2$ and $\zeta = 3$ analogous terms $\rho(D - \mathbf{v}_i \cdot \mathbf{n})\mathbf{v}_i$ and $\rho(D - \mathbf{v}_i \cdot \mathbf{n})v_i^2 / 2$ can be neglected when compared with $\boldsymbol{\sigma}_i \cdot \mathbf{n}$ and $\mathbf{n} \cdot \boldsymbol{\sigma}_i \cdot \mathbf{v}_i$, respectively.

2.5.4 Conservation Equations

Solid Phases

The assumptions on quasistaticity of motion processes and smallness of strains of solid phases allow us to considerably simplify the equation system (2.2). For the solid phases

$$\partial \rho_i / \partial t = 0, \quad (2.90)$$

$$\nabla \cdot \boldsymbol{\sigma}_i = \mathbf{0}, \quad (2.91)$$

$$\rho_i \frac{\partial e_i}{\partial t} = -\nabla \cdot \mathbf{q}_i + \boldsymbol{\sigma}_i : \frac{\partial \boldsymbol{\varepsilon}_i}{\partial t}, \quad (2.92)$$

$$\boldsymbol{\varepsilon}_i = \frac{1}{2} (\nabla \otimes \mathbf{u}_i + (\nabla \otimes \mathbf{u}_i)^T), \quad \mathbf{x} \in V_i, \quad i = a, b, p, l. \quad (2.93)$$

From Eqs. (2.92), (2.82) and (2.7) one can derive the *equation of heat conductivity* for the solid phases

$$\rho_i c_i \frac{\partial \theta_i}{\partial t} = \nabla \cdot (\mathbf{k}_i \cdot \nabla \theta_i) - \alpha_i \theta_i : \frac{\partial \boldsymbol{\sigma}_i}{\partial t} + W_i^*, \quad \mathbf{x} \in V_i. \quad (2.92a)$$

Gas Phase

The assumption on quasistaticity of motion processes allows to write the equation system (2.2) for gas phase in the form

$$\frac{\partial \rho_g}{\partial t} + \nabla \cdot \rho_g \mathbf{v}_g = 0, \quad (2.94)$$

$$\nabla \cdot \boldsymbol{\sigma}_g = \mathbf{0}, \quad (2.95)$$

$$\frac{\partial \rho_g e_g}{\partial t} + \nabla \cdot \rho_g \mathbf{v}_g e_g = -\nabla \cdot \mathbf{q}_g + \nabla \cdot (\boldsymbol{\sigma}_g \cdot \mathbf{v}_g), \quad \mathbf{x} \in V_g. \quad (2.96)$$

Heat conduction equation for the gas phase follows from Eqs. (2.89), (2.94) and (2.96) at $c_g = \text{const}$:

$$\frac{\partial}{\partial t} \rho_g c_g \theta_g + \nabla \cdot \rho_g \mathbf{v}_g c_g \theta_g = \nabla \cdot (k_g \nabla \theta) + \nabla \cdot (\boldsymbol{\sigma}_g \cdot \mathbf{v}_g), \quad \mathbf{x} \in V_g. \quad (2.96a)$$

2.5.5 Conditions on the Phase Interface

For of infinitesimal strains and quasistatic processes the conditions (2.39)–(2.41) on the nondissipative homothermal phase interface without slip are transformed in the following way.

On the surface of contacting gas and i th solid phase there are relations for the jumps of functions:

$$[\rho] D_0 + \rho_g \mathbf{v}_g \cdot \mathbf{n} = \mathbf{0}, \quad [\boldsymbol{\sigma}] \cdot \mathbf{n} = \mathbf{0}, \quad (2.97)$$

$$\rho_i D_0 [e] - \mathbf{n} \cdot \boldsymbol{\sigma}_g \cdot \mathbf{v}_g + \mathbf{n} \cdot [\mathbf{k} \cdot \nabla \theta] = 0,$$

$$[\theta] = 0,$$

$$\mathbf{v}_g \cdot \mathbf{b}_I = 0, \quad \mathbf{x} \in \Sigma_{ig}.$$

For nonreacting phases (for example, gas and pyrolysis residue $i = p$ or gas and filler $i = a$) in the conditions (2.97) the phase transformation rate is $D_0 = 0$.

In addition, *adhesion conditions* are added to the first four conditions (2.97) for viscous gases, where $\mathbf{b}_I$ are the vectors in the surface tangent to the phase interface, which are orthogonal one to another and to the normal vector $\mathbf{n}$, i.e. $\mathbf{n} \cdot \mathbf{b}_I = 0$, $I = 1, 2$.

The conditions are the consequence of compatibility relations (2.44). Really, from (2.44) the Eqs. (2.57) and (2.59) follow, which for the case of infinitesimal strains and the absence of slip can be written in the form

$$\mathbf{v}_g = -\frac{M}{\rho_i}(\mathbf{F}_g \cdot \mathbf{n} - \mathbf{n}) = -D_0 \left(\frac{\rho_i}{\rho_g} - 1 \right) \mathbf{n}, \quad \mathbf{F}_g \cdot \mathbf{n} = \frac{\rho_i}{\rho_g} \mathbf{n}.$$

Multiplying the first equation scalarly by $\mathbf{b}_I$, we derive the condition of adhering (2.97).

At the interface of the i th and j th solid phases the conditions (2.39)–(2.43) under these assumptions for the interface take the form

$$[\mathbf{u}] = 0, \quad [\theta] = 0, \quad \mathbf{x} \in \Sigma_{ij}, \quad (2.98)$$

$$\mathbf{n} \cdot [\boldsymbol{\sigma}] = 0, \quad \rho_i D_0[e] + \mathbf{n} \cdot [\mathbf{k} \cdot \nabla \theta] = 0.$$

For most solid bodies

$$(e_i - e_i^0 - c_i \theta_i) \ll (e_i^0 + c_i \theta_i),$$

so that we may write $[e] = [e^0 + c\theta]$.

To describe the surface ablation one needs the conditions on the phase transformation surface Σ_{ge} for two ideal perfect gases:

$$\mathbf{n} \cdot [\rho \mathbf{v}] = 0, \quad [p] = 0, \quad \rho_g \mathbf{n} \cdot \mathbf{v}_g [I] - \mathbf{n} \cdot [\mathbf{k} \cdot \nabla \theta] = 0. \quad (2.99)$$

Here $[\Omega] = \Omega_g - \Omega_e$ and subscript e corresponds to the external gas medium contacting the gas phase of the composite; speed of the gas phase is much higher than the speed D_0 of the surface motion; $I_g = e_g + (p/\rho_g)$ and $I_e = e_e + (p_e/\rho_e)$ are the enthalpies of the gas media which in accordance with Eqs. (2.88) and (2.89) are expressed by formulae (1.6) and

$$I_g = I_g^0 + \int_0^{\theta_g} \bar{c}_g d\theta = I_g^0 + \bar{I}_g, \quad I_e = I_g^0 + \bar{I}_e, \quad I_g^0 = e_g^0 + \int_0^{\theta_0} c_g d\theta. \quad (2.100)$$

The conditions (2.99) follow from the general relations (2.39)–(2.41) of the phase interface in the framework of quasistatic approximation (i.e. when inertial terms are neglected).

2.5.6 Rate of the Phase Transformation

Let us find an expression for the rate D_0 of phase transformation $i \longrightarrow j$ when the i th phase is solid with infinitesimal strains (for example, polymer resin $i = b$), and the j th phase is a perfect, linear-viscous gas (for example, gaseous pyrolysis products $j = g$).

Expressions (2.63) for chemical potential tensors χ_i of solid and gas phases for this case have the form

$$\chi_i = (\bar{\mu}_i^0 + \psi_i^\theta(\theta_i) + \psi_i^\varepsilon) \mathbf{E} - \frac{\boldsymbol{\sigma}_i}{\rho_i}, \quad (2.101)$$

$$\chi_g = (\bar{\mu}_g^0 + \bar{\psi}_g^\theta(\theta_g) + R\theta_g \ln(p/p^*) \mathbf{E} - \frac{\mathbf{T}'_g}{\rho_g},$$

where

$$\bar{\psi}_g^\theta(\theta_g) = \int_{\theta_0}^{\theta_g} \bar{c}_g d\theta_g - \theta_g \int_{\theta_0}^{\theta_g} \frac{\bar{c}_g}{\theta_g} d\theta_g, \quad (2.102)$$

$$\bar{\mu}_i^0 = \psi_i^0, \quad \bar{\mu}_g^0 = \psi_g^0 + R\theta_0.$$

In accordance with (2.76), the strain gradient $\mathbf{F}_b$ of the solid phase coincides with the unit tensor $\mathbf{E}$; then from the relation (2.57) we can find the expression for the gradient $\mathbf{F}_g$ of the gas phase on the phase interface Σ_{bg} :

$$\mathbf{n} \cdot \mathbf{F}_g \cdot \mathbf{n} = \rho_b / \rho_g. \quad (2.103)$$

For quasistatic processes, the tensors $\mathbf{K}_i$ and $\mathbf{K}_g$ can be neglected when compared with the chemical potential tensors. The surface tension P_Σ can also be neglected, as its influence is usually small for volumetric ablation. Under the assumptions from formulae (2.64) and (2.101) we derive the following equation of type (2.66)

$$\Delta\mu^0 + \Delta\psi^\theta + \Delta\psi_\sigma + R\theta_g \ln(p/p^*) = 0, \quad (2.104)$$

where the following notations are introduced:

$$\Delta\mu^0 = \bar{\mu}_g^0 - \bar{\mu}_i^0, \quad \Delta\psi^\theta = \bar{\psi}_g^\theta - \psi_i^\theta, \quad \Delta\psi_\sigma = \psi_i^\varepsilon + (\sigma_{ni}/\rho_i) + (T'_{gn}/\rho_g),$$

$$T'_{gn} = \mathbf{n} \cdot \mathbf{T}'_g \cdot \mathbf{n}, \quad \sigma_{ni} = -\mathbf{n} \cdot \boldsymbol{\sigma}_i \cdot \mathbf{n}.$$

On resolving the Eq. (2.104) for p , we obtain a relation of type (2.67):

$$p/p^* = \bar{S}_n \equiv \exp\left(-\frac{\Delta\mu^0 + \Delta\psi^\theta + \Delta\psi_\sigma}{R\theta_g}\right). \quad (2.105)$$

On expressing density ρ_g in terms of gas pressure p , we can rewrite the formula (2.103) for the strain gradient $\mathbf{F}_g$ in the form

$$\mathbf{n} \cdot \mathbf{F}_g \cdot \mathbf{n} = \frac{\rho_b R \theta_g}{\bar{S}_n p^*}. \quad (2.106)$$

On substituting the expression $\mathbf{F}_i = \mathbf{E}$ and (2.106) into (2.68), one can find the expression for the rate D_0 of phase transformation ' $i \rightarrow j$ ':

$$D_0 = \left(\frac{p^* \bar{S}_n - \sigma_{ni}}{\rho_i \left(1 - \frac{\rho_i R \theta_g}{p^* \bar{S}_n} \right)} \right)^{1/2}. \quad (2.107)$$

For gas-phase transformations the following conditions are usually satisfied:

$$\Delta\psi^0 \gg \Delta\psi^\theta, \quad \Delta\psi^0 \gg \Delta\psi_\sigma, \quad p^*/(\rho_i R \theta_g) \ll 1,$$

and also $\bar{S}_n \leq 1$. Moreover, one can assume up to a sufficient accuracy that the hydrostatic stress in the solid phase σ_{ni} is equal to the external pressure p_e acting onto the whole composite material, and the pressure p^* is close to the current pressure of the gas phase, i.e.

$$\sigma_{ni} \approx p_e, \quad p^* \approx p. \quad (2.108)$$

Under the assumptions, one can obtain the final expression for rate D_0 of phase transformation ' $i \rightarrow j$ ' from Eq. (2.107):

$$D_0 = D^0 (p/p_e)^{1/2} \exp \left(-\frac{E_A}{R \theta_g} \right) \left(1 - \frac{p}{p_e} \exp \left(-\frac{2E_A}{R \theta_g} \right) \right)^{1/2}, \quad (2.109)$$

$$D^0 = \frac{p_e}{\rho_i (R \theta_g)^{1/2}}, \quad E_A = \Delta\mu^0/2,$$

where E_A is the so-called activation energy of the phase transformation.

The expression (2.109) gives the phase transformation rate D_0 as a function of temperature θ_g and pressure p of the gas phase.

The pressure p appearing in ablative composites usually satisfies the condition

$$\frac{p}{p_e} \exp \left(-\frac{2E_A}{R \theta_g} \right) \ll 1. \quad (2.110)$$

Then the expression (2.109) for the rate D_0 takes the simple form:

$$D_0 = D^0 \exp \left(-\frac{E_A}{R \theta_g} \right). \quad (2.111)$$

The dependence of the phase transformation rate upon temperature θ_g in the form of $\exp(-E_A/(R\theta_g))$ is called *Arrhenius dependence*. As follows from the above conclusion, dependence (2.111) of Arrhenius type takes place only if condition (2.110) is satisfied, i.e. at a relatively low level of temperature θ_g and pressure p . For higher θ_g and p formula (2.109) should be used.

Under infinitesimal strains the Eq. (2.71) describing a location of the phase interface Σ_{ij} takes the form

$$\frac{\partial f_{ij}}{\partial t} + D_0 |\nabla f_{ij}| = 0. \quad (2.112)$$

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