

Cross Effects in Solid-Phase Transformations

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Abstract

The analysis of some cross effects accompanying solid-phase transformations is performed within the frame of the thermodynamics of irreversible processes. Solid-phase systems capable of chemical transformations belong to complicated thermodynamic systems the state of which, unlike the one thermodynamically equilibrium, can be described by introducing additional thermodynamic parameters. Methods of describing additional parameters may be different depending on specific physicochemical situation and required detailing degree. Many cross effects discussed during thermodynamic analysis are known from experiment even if this is not mentioned. Partial models taking account of different cross effects are known in continuum mechanics. Examples are presented that illustrate the principal role of interconnections between different phenomena, which is necessary to take into account in mathematical description of solid-phase transformations.

INTRODUCTION

It is evident that all the real materials obtained and applied in modern technologies are structurally non-uniform. In some cases, one succeeds in describing the properties of these materials on the basis of the ideas of heterogeneous continuum mechanics [1]. Another route, which is suitable, in particular, in modeling the behaviour of solid media containing inner surfaces, pores, cracks, dislocations and other non-homogeneities, involves expansion of modern thermomechanics [2] by introducing additional parameters; methods to describe them may be different [3, 4]. The use of locally equilibrium thermodynamics [5] with additional parameters allows analyzing possible cross effects between various physical and chemical processes observed in solid continuum.

SIMPLE CONTINUUMS

If the components of stresses tensor, temperature and mass concentrations of components are chosen as the basic parameters, Gibbs equation can be represented in the frames of

local-equilibrium thermodynamics [6] as follows:

$$dg = -\varepsilon_{ij} d\sigma_{ij} - s dT + \sum_{(k)} g_k dN_k \quad (1)$$

Here g is local Gibbs potential, g_k are chemical potentials of components, N_k are their mass concentrations, ε_{ij} , σ_{ij} are components of strain and stress tensors, s is local entropy, T is temperature.

The parameters ε_{ij} , s , g_k are also functions of the chosen parameters; each of them can be represented as a full differential. For example,

$$d\varepsilon_{ij} = \sum_{(l,m)} \left(\frac{\partial \varepsilon_{ij}}{\partial \sigma_{lm}} \right)_{T, N_k} d\sigma_{lm} + \left(\frac{\partial \varepsilon_{ij}}{\partial T} \right)_{\sigma, N_k} dT + \sum_{(k)} \left(\frac{\partial \varepsilon_{ij}}{\partial N_k} \right)_{T, \sigma, N_j, j \neq k} dN_k$$

It is known that truly thermodynamic variable is the reaction coordinate x (in the case under consideration, the phase transformation), while the corresponding thermodynamic force is chemical affinity A , which allows us to rewrite (1) in the form [5, 7]

$$dg = -\varepsilon_{ij} d\sigma_{ij} - s dT - A d\xi \quad (2)$$

where

$$g = \sum_{(k)} N_k g_k, \quad A = - \left(\frac{\partial g}{\partial \xi} \right)_{\sigma, E, T, H} = - \sum_{(k)} g_k v_k$$

$$= \sum_{(k)} \left(\frac{\partial g}{\partial N_k} \right) v_k$$

Here n is stoichiometric coefficient, and x actually determines transformation rate (the flux of reaction is its rate)

$$\varphi = \rho \frac{\partial \xi}{\partial t}$$

Here, r is density, t is time. The value $x = 0$ corresponds to the initial state, $x = 1$ would correspond to complete transformation of the reacting substances into reaction products. It is natural that the possibility for transformation to be completed depends on reaction conditions [5]. For r reactions occurring in solid,

$$dg = -\varepsilon_{ij} d\sigma_{ij} - s dT - \sum_{l=1}^r A_l d\xi_l,$$

$$A_l = - \left(\frac{\partial g}{\partial \xi_l} \right)_{\sigma, E, T, H} = - \sum_{(k)} g_k v_{kl}$$

It is evident that

$$d\varepsilon_{ij} = \sum_{(l,m)} \left(\frac{\partial \varepsilon_{ij}}{\partial \sigma_{lm}} \right)_{T, \xi} d\sigma_{lm} + \left(\frac{\partial \varepsilon_{ij}}{\partial T} \right)_{\sigma, \xi} dT$$

$$+ \left(\frac{\partial \varepsilon_{ij}}{\partial \xi} \right)_{T, \sigma} d\xi \quad (3)$$

$$ds = \sum_{(i,j)} \left(\frac{\partial s}{\partial \sigma_{ij}} \right)_{T, \xi} d\sigma_{ij} + \left(\frac{\partial s}{\partial T} \right)_{\sigma, \xi} dT$$

$$+ \left(\frac{\partial s}{\partial \xi} \right)_{T, \sigma} d\xi \quad (4)$$

$$dA = \sum_{(i,j)} \left(\frac{\partial A}{\partial \sigma_{ij}} \right)_{T, \xi} d\sigma_{ij} + \left(\frac{\partial A}{\partial T} \right)_{\sigma, \xi} dT$$

$$+ \left(\frac{\partial A}{\partial \xi} \right)_{T, \sigma} d\xi \quad (5)$$

The A value can be determined with the help of any one of thermodynamic potentials [5]. In the case under consideration, the equation $dg = 0$ corresponds to the thermodynamic equilibrium condition. Hence, under equilibrium conditions at constant temperature and stress, $A = 0$ and equilibrium reaction coordi-

nate depends on temperature and stress-strained state of the system:

$$\xi_e = \xi_e(T, \sigma_{ij})$$

The matrix of the coefficients of the system of equations (3)–(5) described cross (direct and reverse) first-order effects that are principally possible in the thermodynamic system under consideration. Derivatives

$$s_{lmij} = \left(\frac{\partial \varepsilon_{ij}}{\partial \sigma_{lm}} \right)_{T, \xi} = - \left(\frac{\partial^2 g}{\partial \sigma_{lm} \partial \sigma_{ij}} \right)_{T, \xi}$$

are the components of the tensor of elastic compliance coefficients; derivatives

$$\frac{c_\sigma}{T} = \left(\frac{\partial s}{\partial T} \right)_{\sigma, \xi} = - \left(\frac{\partial^2 g}{\partial T^2} \right)_{\sigma, \xi}$$

actually define specific heat at constant strain; the coefficient

$$\left(\frac{\partial A}{\partial \xi} \right)_{T, \sigma} = - \left(\frac{\partial^2 g}{\partial \xi^2} \right)_{T, \sigma} = - \sum_{(k)} v_k \left(\frac{\partial^2 g}{\partial \xi \partial N_k} \right)_{N_l, T, \sigma}$$

determines the extent to which chemical affinity depends on reaction coordinate. If the tensors of stress and strains are symmetrical, we can write the following equation for the cross terms describing cross effects:

$$\left(\frac{\partial A}{\partial \sigma_{ij}} \right)_{T, \xi} = \left(\frac{\partial \varepsilon_{ij}}{\partial \xi} \right)_{T, \sigma} = - \left(\frac{\partial^2 g}{\partial \sigma_{ij} \partial \xi} \right)_T$$

$$= - \sum_{(k)} v_k \left(\frac{\partial^2 g}{\partial \sigma_{ij} \partial N_k} \right)_{T, N_l}$$

$$\left(\frac{\partial s}{\partial \sigma_{ij}} \right)_{T, \xi} = \left(\frac{\partial \varepsilon_{ij}}{\partial T} \right)_{\sigma, \xi} = - \left(\frac{\partial^2 g}{\partial \sigma_{ij} \partial T} \right)_\xi \quad (6)$$

$$\left(\frac{\partial A}{\partial T} \right)_{\sigma, \xi} = \left(\frac{\partial s}{\partial \xi} \right)_{T, \sigma} = - \left(\frac{\partial^2 g}{\partial T \partial \xi} \right)_\sigma$$

$$= - \sum_{(k)} v_k \left(\frac{\partial^2 g}{\partial T \partial N_k} \right)_{\sigma, N_l}$$

In accordance with the thermodynamics of irreversible processes, transformation rate is determined by chemical affinity, *i. e.*,

$$\frac{\partial \xi}{\partial t} = L \frac{A}{T} \quad (7)$$

Here L is phenomenological coefficient. For small deviations from equilibrium at $s_{ij} = \text{const}$, $T = \text{const}$, one can write [5]:

$$A = \left(\frac{\partial A}{\partial \xi} \right)_{\sigma, T} \Delta \xi = - \left(\frac{\partial^2 g}{\partial \xi^2} \right)_{\sigma, T} \Delta \xi \quad \Delta \xi = \xi - \xi_e$$

Hence, we obtain from (7)

$$\frac{\partial \xi}{\partial t} = - \frac{\xi - \xi_e}{\tau_{T, \sigma}}$$

$$\text{Here } \tau_{T, \sigma} = \frac{\rho T}{L \cdot \left(\partial^2 g / \partial \xi^2 \right)_{T, \sigma}} > 0 \text{ because } L > 0 \text{ due}$$

to the positive determinacy of entropy production; $\partial^2 g / \partial \xi^2 > 0$ because Gibbs energy has a minimum under the equilibrium conditions at constant stresses and temperature. Thus, near the equilibrium, ξ tends to its equilibrium value following the exponential law.

Taking account of (6), we can indicate as a first approximation what factors affect the transformation rate and the time within which the thermodynamic system relaxes to its equilibrium state. In a simple thermodynamic system, the transformation can cause strains, release of absorption of heat. In turn, stresses and strains affect reaction rate by changing chemical affinity or chemical potentials of the components participating in the reaction. Thus, cross effects of feedbacks between different physical phenomena are observed also in a simple thermodynamic system.

The role of cross effects in describing real processes in solids during production and treatment of materials can be principal. They get special importance in the kinetics of solid-phase transformations since they are the channels along which the external factors can affect transformation rate [8–10].

COMPLICATED MEDIA

To describe complicated thermodynamic media [11, 12], to which structurally non-uniform materials belong, it is necessary to broaden the set of thermodynamic variables determining the state of the system. Within the frame of local-equilibrium thermodynamics, one should speak of the state at a given moment of time in a given point of space; all the variables that are introduced (generalized thermodynamic coordinates) should be additive. Assuming that the independent variables are tempera-

ture and the components of strain tensor, we can write down the Gibbs' equation for the local Gibbs' energy as

$$dg = -s dT - \varepsilon_{ij} d\sigma_{ij} - A d\xi - \sum_{(k)} B_k db_k \quad (8)$$

Then,

$$d\varepsilon_{ij} = \left(\frac{\partial \varepsilon_{ij}}{\partial T} \right)_{\sigma, b, \xi} dT + \left(\frac{\partial \varepsilon_{ij}}{\partial \sigma_{lm}} \right)_{T, b, \xi} d\sigma_{lm} + \left(\frac{\partial \varepsilon_{ij}}{\partial \xi} \right)_{T, \sigma, b} d\xi + \left(\frac{\partial \varepsilon_{ij}}{\partial b_k} \right)_{T, \sigma, \xi} db_k \quad (9)$$

$$ds = \left(\frac{\partial s}{\partial T} \right)_{\sigma, b, \xi} dT + \left(\frac{\partial s}{\partial \sigma_{ij}} \right)_{T, b, \xi} d\sigma_{ij} + \left(\frac{\partial s}{\partial \xi} \right)_{\sigma, b, T} d\xi + \left(\frac{\partial s}{\partial b_k} \right)_{T, \sigma, \xi} db_k \quad (10)$$

$$dB_k = \left(\frac{\partial B_k}{\partial T} \right)_{\sigma, b, \xi} dT + \left(\frac{\partial B_k}{\partial \sigma_{ij}} \right)_{T, b, \xi} d\sigma_{ij} + \left(\frac{\partial B_k}{\partial \xi} \right)_{\sigma, b, T} d\xi + \left(\frac{\partial B_k}{\partial b_n} \right)_{T, \sigma, \xi} db_n \quad (11)$$

$$dA = \left(\frac{\partial A}{\partial T_{ij}} \right)_{\sigma, b, \xi} dT + \left(\frac{\partial A}{\partial \sigma_{ij}} \right)_{T, b, \xi} d\sigma_{ij} + \left(\frac{\partial A}{\partial \xi} \right)_{\sigma, b, T} d\xi + \left(\frac{\partial A}{\partial b_k} \right)_{T, \sigma, \xi} db_k \quad (12)$$

This means that the change of entropy is possible as a consequence of the change of any of the thermodynamic parameters; strains can appear as a consequence of various processes connected with the changes of additional parameters; all the components of the vector of generalized forces depend on temperature, components of the tensor of stress and various thermodynamic variables, and on the reaction coordinate (the properties of substance being naturally changed during this reaction). The time of reaction relaxation to the equilibrium state under the considered conditions now will be

$$\tau_{T, \sigma} = \frac{\rho T}{L \left(\partial^2 g / \partial \xi^2 \right)_{T, \sigma, b}} > 0$$

Let us choose the following additional variables (besides mass concentrations of components able to undergo chemical and phase transformations): area of inner surfaces, specific

volume of non-uniformities (cracks, pores, voids), density of dislocation distribution, and concentration of vacancies. The corresponding thermodynamic forces will be: surface energy, potential of non-uniformities (or energy which is necessary for their formation due to rupture of chemical or molecular bonds), potentials of dislocations and vacancies, similar in sense to chemical potentials of components. Any of the newly introduced values meets the requirement of balance equation. As usual equations of mass, pulse, energy and pulse momentum conservation (balance), additional conservation equations are written down in local and substantial forms [5, 6]. Fluxes of all the elements of structure (defects: inner surfaces, vacancies, dislocations, non-uniformities) depend on diverse thermodynamic forces. The corresponding equations are written with the help of Onsager's theory or its generalization for non-equilibrium processes. All the mentioned general statements are known but they are not always correctly used in building up specific models. A principal moment of such an approach is the mutually dependent character (connection) of resulting equations, which depicts mutually determined character of real physical and chemical processes. In particular, taking account of the connection character of different processes one can write down the explicit matrix of thermodynamic properties of crystals [13] and indicate the routes by which external factors affect rates and directions of local processes including phase and chemical transformations in a solid continuum. Internal connections between different processes are observed independently of the type of external action and of whether external action is present or not.

It follows from (8) and (9)

$$\left(\frac{\partial \varepsilon_{ij}}{\partial b_k}\right)_{T,\sigma} = -\left(\frac{\partial^2 g}{\partial b_k \partial \sigma_{ij}}\right)_T$$

while (8) and (11) suggest

$$\left(\frac{\partial B_k}{\partial \sigma_{ij}}\right)_{T,b} = -\left(\frac{\partial^2 g}{\partial \sigma_{ij} \partial b_k}\right)_T$$

If tensors of stresses and strains are symmetrical, we can write

$$\beta_{ij}^{(k)} = \left(\frac{\partial \varepsilon_{ij}}{\partial b_k}\right)_{T,\sigma} = \left(\frac{\partial B_k}{\partial \sigma_{ij}}\right)_{T,b} \quad (13)$$

This means that the change of strains tensor components at varying thermodynamic parameter b_k is described by the same coefficients as the change of potential B_k under the action of stresses. Similarly,

$$a_k = \left(\frac{\partial B_k}{\partial \xi}\right)_{T,\sigma,b} = \left(\frac{\partial A}{\partial b_k}\right)_{\sigma,T,\xi} \quad (14)$$

which means that the change of thermodynamic force B_k in course of reaction is equal to the change of the affinity of this reaction at the corresponding variation of the generalized parameter b_k .

From the viewpoint of the thermodynamics of irreversible processes, the equations (3), (9) are linearized equations of state. In a particular case of isotropic medium, it follows from (9)

$$dv = v_p dp + v_T dT + v_\xi d\xi + \sum_{(k)} v_k db_k \quad (15)$$

Here v_p , v_T , v_x , v_k are volume changes caused by local changes of pressure, temperature, and other thermodynamic variables.

Some particular cases of (3) and (9) are known in mechanics. For example, assuming $db_k = 0$ we obtain

$$d\varepsilon_{ij} = s_{ijlm} d\sigma_{lm} + \alpha_{ij} dT \quad (16)$$

$$ds = \alpha_{ij} d\sigma_{ij} + \frac{c_s}{T} dT \quad (17)$$

Here α_{ij} are components of the tensor of heat expansion coefficients; c_s is specific heat at constant stresses. In fact, equations (17) are usual Duamel – Neumann equations in the differential form. Then, (9) will be their generalization for the case when irreversible processes of different kinds occur in the medium causing irreversible strains. Using (16), (17) and usual equations of mass, energy, pulse, pulse moment conservation we arrive at the system of coupled equations of thermal elasticity theory.

Assuming $db_k = 0$, $dT = 0$ we obtain:

$$d\varepsilon_{ij} = s_{ijlm} d\sigma_{lm} + \sum_{(k)} \alpha_{ij}^{(k)} dN_k \equiv s_{ijlm} d\sigma_{lm} + \alpha_{ij}^{(\xi)} d\xi \quad (18)$$

while $\alpha_{ij}^{(\xi)} = -\sum_{(k)} \alpha_{ij}^{(k)} v_k$. This equation brings

together the components of the tensors of stresses and strains, which are the consequences of diffusion in solid medium or of physicochemical transformations; the use of mass concentrations of components or reaction coordinates as thermodynamic variables of state is equivalent. The coefficients $\alpha_{ij}^{(k)}$ describe phenomena in the interaction of the fields of strain and concentrations; in literature, for example, in [14], the latter coefficients are related to as concentrational expansion coefficients over k -th components, or dilatancy coefficients. They can be calculated on the basis of elementary notions. The $\alpha_{ij}^{(\xi)}$ coefficients depict the fact that strains arise as a result of reaction, or the change of its affinity under the action of internal stresses.

An example with solid-phase diffusion is less usual in the models of mechanics, though it has many applications to problems arising in the production of materials when their surface physicochemical treatment is performed. Modeling of diffusion in solid media, including the effect of internal stresses and strains, and estimations of strain resulting from non-uniformities of concentration fields are the subject of many publications, for example [14–18]. The known theories include: isothermal multicomponent diffusion taking account of crossover fluxes of components, equilibrium and non-equilibrium fluxes of vacancies; partial models of diffusion in the field of structural non-uniformities, *etc.* In real media, mechanisms and rate of diffusion may be different, which is determined not only by external conditions but also by the structure of the medium. In particular, the rate of diffusion in solid crystal volume may differ by several orders of magnitude from that along the boundaries of grains and phases. A special thermodynamic analysis of mutual diffusion in volume and over boundaries was performed in [19].

Similarly to (18), taking $dT = 0$ and considering specific area of inner surfaces as an additional thermodynamic parameter one can write down:

$$d\varepsilon_{ij} = s_{ijkl} d\sigma_{kl} + \sum_{(k)} \alpha_{ij}^{(k)} dN_k + \alpha_{ij}^{(s)} df_s \equiv s_{ijkl} d\sigma_{kl} + \alpha_{ij}^{(\xi)} d\xi + \alpha_{ij}^{(s)} df_s \quad (19)$$

$$dA = -\alpha_{ij}^{(\xi)} d\sigma_{ij} + \left(\frac{\partial A}{\partial \xi} \right)_{\sigma, f_s} d\xi + \left(\frac{\partial A}{\partial f_s} \right)_{\sigma, \xi} df_s$$

$$dg_s = -\alpha_{ij}^{(s)} d\sigma_{ij} + \left(\frac{\partial g_s}{\partial \xi} \right)_{\sigma, f_s} d\xi + \Omega df_s$$

Here the first terms in the generalized equation describe reversible strains while others relate to irreversible ones; the $\alpha_{ij}^{(s)}$ coefficients describe cross phenomena (likely to be observed experimentally) in the interaction of inner surfaces with the stresses field. The parameter W depicts local change of specific surface energy with changing area. Similarly, change of the affinity of chemical reaction (or its rate) at the change of f_s parameter is described by the same coefficient as the change of specific surface energy during chemical reaction is. The dependence of the rate of reaction in solid phase on the area of inner surfaces is indisputable fact in solid state chemistry [20]. Similarly we may indicate the routes by which various defects affect transformation rates [21] and formation of internal stresses and strains [3, 4].

In the simplest case, the equation (7) is correct for the rate of chemical reaction; however, now chemical affinity depends on a large number of thermodynamic variables of state. In the general case, one should take account of the occurrence of scalar processes of another type (different from chemical reaction itself) in the thermodynamic system. For example, processes that occur in a solid include the formation and multiplication of dislocations and microdefects, changes of the area of inner surfaces, formation or collapse of microcracks, pores, voids as a result of destruction in the reaction region under the action of internal strain, *etc.* These processes involve their own sources and sinks in conservation (balance) equations. Hence, one can write instead of (7)

$$\Phi = L \frac{A}{T} + \sum_{(k)} L_k' \frac{B_k}{T} \quad (20)$$

Generally speaking, the linear approximation (7) is true only for reactions that occur

under the conditions not far from the equilibrium ones. It is probable that taking account of cross effects one would be able to broaden the range of parameters in which the application of linear laws will give suitable results. Besides, on the basis of the methods of modern thermodynamics of irreversible processes, generalization for Onsager's equations may be proposed which would be correct for non-equilibrium processes, and also other theories may be built up [2-4, 22].

Thus, the model of real solid-phase chemical reaction should be coupled, *i. e.* it should be described by equations containing both direct and reverse effects.

EXAMPLES OF COUPLED MODELS

In order to illustrate the above conclusion, let us describe simple examples of calculations based on coupled models of solid-state transformations.

A coupled model of the development of the solid-phase reaction nucleus is proposed in [23] taking account of various physical processes (deformation, accumulation of damages, changes of properties during transformations); different transformation modes are investigated; critical conditions that divide them from each other are determined depending on parameters. Unlike classical works in the area of mechanics dealing with the analysis of irreversible strains, this model does not introduce explicitly the yield stress that gives a limitation for stresses. Nevertheless, strains that accompany a solid-phase reaction are irreversible. Results obtained in [23] demonstrate that there is no necessity to introduce limitations of achievable stresses in the coupled model. The components of the tensors of stresses and strains in the coupled model are connected by relations like (19) where f_s is understood as specific volume of damages, or damage factor, while a_s coefficient at f_s is called structural expansion coefficient (it is scalar in the model of isotropic continuum). If $a_s = 0$, stresses and strains reach very large values in the substance along the direction in which the reaction propagates from the initial nucleus. Specific volume of damages can also reach unreal values (1 when

measured in relative units). Assuming $a_s \neq 0$ we obtain real physical values and relaxation of strain if the properties change insignificantly during transformation. Taking account of the changes of properties during reaction we obtain residual stresses by calculations.

The investigation of such a model within a broad range of the changes of parameters (without taking account of destruction) leads to one more interesting result [24], namely, periodic regimes of transformation. Within some range of the changes of parameters, mass transfer under the action of strain gradient plays a substantial part. This is exhibited as the transfer in the positive direction of concentration gradient. Mathematical formulation of the problem taking account of the effect of stresses on the transfer of substance can be represented in the form

$$\frac{\partial y}{\partial \tau} + \varphi(y) = \frac{1}{\delta} \frac{\partial^2 y}{\partial \xi^2} [1 - By] + \frac{1}{\delta} \left[\frac{2}{\xi} - B \left(\frac{2}{\xi} y + \frac{\partial y}{\partial \xi} \right) \right] \frac{\partial y}{\partial \xi}$$

$$\tau = 0 : \begin{cases} y = y_0, & |\xi| \leq 1 \\ y = 0, & |\xi| > 1 \end{cases}$$

$$\xi = 0, \infty : \partial y / \partial \xi = 0$$

Here x is spatial coordinate divided by the initial radius of a nucleus, τ is dimensionless time, d and B are dimensionless parameters of the problem, y_0 is initial fraction of reaction product in the nucleus, y is transformation degree.

At small B values, the reaction develops from the initial nucleus in the diffusion mode; at rather large B the reaction development is periodic in character, the reaction is not completed in any point of the substance; regions of variable configuration are formed in the volume of the substance. It is likely that incomplete transformation in reaction, periodic structures, various oscillating phenomena in solid-phase processes, instabilities and threshold effects originate from cross effects; theoretical considerations in literature pay unreasonably poor attention to them.

By the way, different steady transformation regimes connected with the effect of mechanical processes on the transfer of substance have been discovered also in a more complicated model for the reaction of the type $A_s + B_s = C_s$ [25] (an example of such a

reaction is the formation of spinels); the only possible rate constant for the growth of cracks that would provide joint propagation of the fronts of reaction and destruction has been stated for the coupled model of dehydration [26].

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