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MECHANOTHERMODIFFUSION PROCESS IN LOCALLY HETEROGENEOUS MULTI COMPONENT MEDIA

Summary. By means of non-equilibrium thermodynamics and continuum mechanics methods we have got an initial system of mechanothermodiffusion equations with account to heat conduction and admixture diffusion in two ways corresponding to different local states of the body components with heat exchange and transition of particles between them.

MECHANOTERMODYFUZYJNE PROCESY W LOKALNIE NIEJEDNOLITYCH WIELOSŁADOWYCH ŚRODOWISKACH

Streszczenie. Wykorzystując metody nierównowaznej termodynamiki oraz mechaniki zwartego środowiska otrzymano wyjściowy system równań mechanotermodyfuzji z uwzględnieniem przewodnictwa cieplnego i dyfuzji domieszki dwoma sposobami, odpowiadającymi różnym lokalnym stanom składowych ciała przy wymianie ciepła i cząstek między nimi.

О МЕХАНОТЕРМОДИФФУЗИОННЫХ ПРОЦЕССАХ В ЛОКАЛЬНО- НЕОДНОРОДНЫХ МНОГОКОМПОНЕНТНЫХ СРЕДАХ

Резюме. Методами неравновесной термодинамики и механики сплошной среды получена исходная система уравнений механотермодиффузии, учитывающая теплопроводность и диффузию примеси двумя путями, которые соответствуют различным локальным состояниям компонент тела при теплообмене и переходе частиц между ними.

1. INTRODUCTION

In the existing models of continuum media mechanics the mechanical behaviour and other properties of multicomponents finely dispersed bodies are described, as a rule, by using the approach of solid solution [1, 2] or the conceptions of multivelocity continuum theory [3]. But within the framework of these approaches it is not always possible to take exactly into account the influence of local changes in compound components and the body phases which occur in the processes like phase transitions. The initial system of mechanical thermodiffusion equations which takes into account thermoconductivity and admixture diffusion in two ways corresponding to different local states of body component at heat exchange and participle transition between them has been obtained by means of thermodynamics of irreversible processes using continuous conception.

Let a small and arbitrarily chosen region of the body consist of solid and liquid phases and admixture particles of one type. Within each phase admixture particles are in essentially different [physical states (one or more than one). Under external influence non only thermoconductivity processes, but also diffusion, heat and mass exchanges between above mentioned phases take place in the body. Deformation process is described using continuous conception. Continua M_{s1} and M_{s2} are compared with the particles forming the solid phase and the admixture substances in it, and centre mass continuum M_1 is compare with the subsystem as a whole. In a similar way continua M_{l1} , M_{l2} and M_1 are considered for the liquid subsystem.

2. LOCAL STATE

To determine specific value for field description of the system and formulate different kinds of boundary conditions it is necessary to agree with the choice and to specify the extensive and intensive properties of macroscopic parameters determining the local thermodynamic states of the solid and liquid subsystems. It should be noted that Gibb's equation for close subsystems [4, 5], introduced here is as follows:

$$dU_i = T_r ds_i - P_i dV_r, \quad dU_s = T_s dS_s + \frac{1}{2} V_s \sigma_s^{ij} dg_{ij}^{(s)}, \quad (1)$$

where U_r is internal energy, T_r is absolute temperature, S_r is entropy, V_r is volume, σ_s^{ij} and $g_{ij}^{(s)}$ are Cauchy stress tensor components and metric tensor; P_i is the pressure ($\bar{\sigma}_i = -P_i \bar{I}$, \bar{I} is unit tensor), $r = \overline{s, l}$. The values $S_r(am_r) = aS_r(m_r)$, $V_r(am_r) = aV_r(m_r)$, $U_i(am_i) = a U_i(m_i)$ and also $U_s(aS_s, V_s^{2/3} g_{ij}^{(s)}, am_s) = aU_s(S_s, g_{ij}^{(s)}, m_s)$, have extensive natural properties, where m_r is the mass of subsystem r , $a > 0$ is a certain number. Taking into consideration a potential character of internal energy U_r , coordination of Euler equation for the solid and liquid subsystems and introducing specific values we write

$$du_l = T_l ds_l - P_l \rho_l^{-1} + \sum \mu_{lk} dC_{lk}$$

$$du_s = T_s ds_s + \frac{1}{2} \rho_s^{-1} \sigma_s^y d g_{ij}^{(s)} + \sum \mu_{sk} dC_{sk}, \quad k = \overline{1,2}, \quad (2)$$

Here $\mu_{lk} = (\partial U / \partial m_{lk})_{s, v_l, m_{l \neq k}}$ is the chemical potential of k component in the liquid subsystem, $\mu_{sk} = \mu_{sk} + \frac{1}{2} (g_s \dot{g}_s^{-1})^{1/2} v_{sk} \sigma_s$ is an overstandartized chemical potential of k component in the solid subsystem, $\mu_{sk} = (\partial U_s / \partial m_{sk})_{s, v_s, g_{ij}, m_s}$ is its initial chemical potential, $\sigma_s = \sigma_s^y g_{ij}^{(s)}$ is the first invariant of Cauchy stress tensor, $V_{sk}^* = (\partial V_s^* / \partial m_{sk})_{T_s, \sigma_s^y, m_{l \neq k}}$ is specific partial volume of k components, $C_{rk} = m_{rk} / (m_{r1} + m_{r2})$ is the mass component concentration, g and \dot{g} are determinants of metric tensor in deformed and initial states ($n, k = \overline{1,2}$). In this case Euler equation is as follows

$$T_l s_l - P_l \rho_l^{-1} + \sum \mu_{lk} c_k = u_l, \quad T_s s_s + \frac{1}{3} \sigma_s \rho_s^{-1} + \sum \mu_{sk} C_k = u_s \quad (3)$$

and the values

$$T_l - S_p, \quad P_l - V_p^*, \quad T_s - S_s, \quad V_s^{*1/3} \sigma^y - V_s^{*2/3} g_{ij} \quad (4)$$

have necessary intensive and extensive properties for coordinated description of the solid and liquid subsystems. By means of Gibb's potential $g_l = u_l - T_l s_l + P_l \rho_l^{-1}$ and $g_s = u_s - T_s s_s - \frac{1}{3} \sigma_s \rho_s^{-1}$ from (2) - (4) formulas the state equations may be found

$$s_l = s_l(T_l, P_l, C_p, C_{l2}), \quad v_l = v_l(T_l, P_l, C_p, C_{l2}),$$

$$\mu_{lk} = \mu_{lk}(T_l, P_l, C_{l1}, C_{l2}), \quad (v_l = \rho_l^{-1});$$

$$s_s = s_s(T_s, \sigma_s^y, C_{s1}, C_{s2}), \quad g_{ij}^{(s)} = g_{ij}^{(s)}(T_s, \sigma_s^y, C_{s1}, C_{s2}),$$

$$\mu_{sk} = \mu_{sk}(T_s, \sigma_s^y, C_{s1}, C_{s2}) \quad k = \overline{1,2}. \quad (5)$$

3. BALANCE EQUATIONS

While irreversible processes take place in the system changes in extensive parameters must obey the laws of mass, impulse and energy conservation. In this case the law of mass conservation is reduced to the following equation for the total density of the following subsystems

$$\frac{\partial \rho_l}{\partial t} + \bar{\nabla} \cdot (\rho_l \bar{v}_l) = -J, \quad \frac{\partial \rho_s}{\partial t} + \bar{\nabla} \cdot (\rho_s \bar{v}_s) = J \quad (6)$$

and admixture concentration there

$$\rho_l \frac{d_l C_l}{dt} = -\bar{\nabla} \cdot \bar{J}_l - J(1-C_l), \quad \rho_s \frac{d_s C_s}{dt} = -\bar{\nabla} \cdot \bar{J}_s + J(1-C_s), \quad (7)$$

where $\bar{v} = (\rho_{r1} \bar{v}_{r1} + \rho_{r2} \bar{v}_{r2}) / \rho_r$, is the velocity of points in mass centre continuum compared to the subsystem r ; J is the scalar flux of particles (production or source) from the liquid subsystem into the solid one; $d/dt = \partial/\partial t + \bar{v}_r \cdot \bar{\nabla}$, $\bar{\nabla}$ is Hamilton operator; \bar{J} are vector mass fluxes of admixture substance; $C_r = C_{r2}$, $\rho_r = (\rho_{r1} + \rho_{r2})$, ($r = l, s$)

Analysing local state of the subsystem the law of impulse conservation can be written as follows taking into account already used expression for work:

$$\rho_r \frac{d_r \bar{v}_r}{dt} = \bar{\nabla} \cdot \hat{\sigma}_r + \rho_r \bar{g}_r \pm \bar{P} \pm J \bar{v}_s, \quad r = \bar{l}, s, \quad (8)$$

where \bar{g}_r is mass potential and conservation forces (like gravity), \bar{P} is vector of force interaction in the subsystem ($\hat{\sigma} = -p_l \hat{I}$).

Using the total energy conservation law a balance equation for internal energy is obtained from the laws of potential and kinematic energy conservation which are the result of equations (6) and (8). Comparing it with the corresponding Gibb's equation (2) we find balance correlations for subsystems entropies. Examining local system region on the whole we can write the following balance entropy equation for it:

$$\rho_l \frac{d_l S_l}{dt} + \rho_s \frac{d_s S_s}{dt} = \bar{\nabla} \cdot \bar{J}^s + Q^{(a)}, \quad (9)$$

where \bar{J}^s is the entropy flux, which is determined by the proper heat fluxes in the subsystem, $Q^{(a)}$ is its production.

4. KINETIC EQUATION

Entropy production $Q^{(e)}$ is a polynear form of product of thermodynamic fluxes and forces, being gradients of the corresponding intensive parameters or difference for the given subsystems or their combination. Considering fluxes as function of the following thermodynamic forces and taking into account Onzager principle [6] kinetic potential Φ is introduced. Its differential is

$$d\Phi = J_\lambda dY_\lambda, \quad (10)$$

where J_λ and X_λ are thermodynamic fluxes and forces (index λ marks scalar values and components of vector or tensor values). At the known functional dependence $\Phi(X_1, \dots, X_n)$ kinetic correlations can be found from the expression (10)

$$J_\lambda = J_\lambda(X_1, \dots, X_n). \quad (11)$$

With account to the state equation (5) and expressions for thermodynamic forces

$$\begin{aligned} X_t &= 1/T_t - 1/T_s, & X_\mu &= \mu/JT_t - \mu/Jt_s, & \bar{X}_v &= \bar{v}/JT_t - \bar{v}/Jt_s, \\ \bar{X}_{rT} &= -\bar{\nabla}T/JT_r, & \bar{X}_{\mu r} &= -\bar{\nabla}\mu_r, & r &= \bar{l}_s. \end{aligned} \quad (12)$$

(without viscosity effects) these correlations allow to obtain the key system of equations from balance correlations (7) - (9) to find stress - deformation state, concentration fields and temperature.

5. CONCLUSION

The presented approach has been used to determine concrete models of mechanical heterodiffusion in two ways in a medium with traps and electrical mechanodiffusion. A number of properties of mass transfer process in finely dispersed media has been investigated and the corresponding calculation schemes have been constructed.

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