THERMO-MECHANICAL PROPERTIES OF MAGNESIA CARBON FOAM COMPOSITES

A. Jung^{*} and S. Diebels^{*}

*Lehrstuhl für Technische Mechanik Universität des Saarlandes Campus A4 2, 66123 Saarbrücken, Germany e-mail: anne.jung@mx.uni-saarland.de, web page: http://www.ltm.uni-saarland.de

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Abstract. Refractory materials have a wide range of applications in steel-making industry. Often, magnesia carbon bricks (MgO-C) are used. These consist of a periclase phase (MgO) with inclusions of carbon and gas filled pores. The thermo-mechanical properties of MgO-C composites could significantly be improved using cellular MgO-C composites based on carbon foams. Modelling of MgO-C composite foams is not only a multi-phase, but also a multi-physics problem, in which both the displacement field and the temperature field have to be taken into account. In the present contribution, a fully coupled phenomenological thermo-mechanical continuum model was developed. The theory of porous media (TPM) with a kinematic coupling of the displacement and temperature fields of all constituents was used. Linear thermoelasticity with a multiplicative decomposition of the deformation gradient into an elastic and a thermal part for isotropic materials was extended to the mixture of MgO and C phase. The total macroscopic stress was calculated using the theory of mixture, including the contributions from the pore pressure.

1 INTRODUCTION

Refractory materials have a wide range of applications in steel-making industry as lining of furnaces, oxygen converters or for ladles. Common refractories are made of a periclase phase (MgO) with inclusions of carbon and gas filled pores. In their applications, refractories are subjected to thermal and mechanical loads causing damage. There are two possible types of thermally induced stress. Permanent thermal stress arises only in heterogeneous materials due to the coupling of materials having different coefficients of thermal expansion (CTE). The corresponding thermal damage results from the isotropic expansion of both phases. Temporary thermal stresses emerge by temperature gradients in homogeneous and also in heterogeneous materials causing mechanical damage and vanish for elastically loaded materials at thermal equilibrium. Mechanical damage occurs not only in multi-phase materials with differences in their CTE but also in homogeneous single phase materials. In the quasi-static heating of a furnace, no temperature gradients arise, hence the only possible thermal stresses are permanent thermal stresses due to the coupling of materials with a mismatch in their CTEs.

The next generation of carbon containing refractories should show improved characteristics in terms of microstructural design, material processing, and material sustainability. In recent studies, the thermo-mechanical properties of MgO-C composites could significantly be improved using cellular MgO-C composites based on carbon foams [1]. Foams consist of three different hierarchical levels. The macro scale deals with whole components, the meso scale with several pores and the micro level comprises single struts. In experiments and modelling, foams can be described on these different scales.

Modelling of MgO-C composite foams is not only a multi-phase and multi-physics problem, but also a multi-scale problem. In previous work, a mesoscopic elastic thermomechanically coupled model was used to investigate the structure-property relationship of MgO-C hybrid foams, in order to reduce thermally induced stresses and accompanying damage [2]. In the present contribution, the thermo-mechanical behavior of cellular ceramic composites will be modelled by a new multiphase approach of porous media using a fully coupled phenomenological thermo-mechanical continuum model. The key assumption is the use of the theory of porous media (TPM) with a kinematic coupling of the displacement and temperature fields of all constituents.

2 KINEMATICS FOR MgO-C FOAMS BY A MULTIPHYSICS APPROACH

Figure 1 shows the typical repesentative elementary volume (REV) of the micro structure of a common MgO-C brick and of a cellular MgO-C foam. Whereas common MgO-C bricks consist of a carbon matrix with inclusions of MgO and irregular pores, the new MgO-C foams consit of a carbon skeleton and more or less circular pores. The carbon skeleton is coated with a layer of MgO. There are several ways to model such problems. On the one hand, each constituent can be modeled according a single phase theory. Due to the coupling and contact of the constituents, this is very expensive. For each micro structure a different approach is needed. On the other hand, both micro structures can be described and modelled using the TPM by homogenization of the mixture and solving the problem as smeared out multiphase continuum. The theory of mixture according to Truesdell & Topin [3] uses a continuum with statistically distributed, immiscible constituents, but there is not a volumetric measure of the constituents included. Hence, for porous media, the concept of volume fractions can be introduced [4].

According to the concept of volume fractions, the volume V of the body \mathcal{B} is the sum of the partial volumes V^{β} of the constituents φ^{β} in the body \mathcal{B} . In the case of the MgO-C foams, a volume element dv of the mixtures consists of the sum of the partial volume elements dv^{β} of all phases φ^{β} . Here, the three constituents carbon (φ^{1}), magnesia (φ^{2})



Figure 1: REV of a common MgO-C brick (a) and of a new cellular MgO-C foam (b) and substitute model according to the concept of volume fractions (c).

and pore gas (φ^3) are taken into account.

$$dv = dv^{1} + dv^{2} + dv^{3} = \sum_{\beta=1}^{k} dv^{\beta} \quad \text{for} \quad k = 1, 2, 3 \tag{1}$$

$$V = \int_{\mathcal{B}} \mathrm{d}v = \sum_{\beta=1}^{k} V^{\beta} \quad \text{with} \quad V^{\beta} = \int_{\mathcal{B}} \mathrm{d}v^{\beta} = \int_{\mathcal{B}} n^{\beta} \,\mathrm{d}v \quad \text{and} \quad n^{\beta} = \frac{\mathrm{d}v^{\beta}}{\mathrm{d}v} \quad (2)$$

The volume fraction n^{β} is the local quotient of the volume element dv^{β} of φ^{β} referred to the volume element dv of the mixture. The volume fractions of all constituents must fulfill the saturation condition, whereas the sum of all volume fractions is equal one. Hence, the volume fraction of one phase can be calculated from the volume fractions of the other phases

$$\sum_{\beta=1}^{k} n^{\beta} = 1 \quad \text{with} \quad k = 1, 2, 3 \quad \text{hence,} \quad n_1 + n_2 + n_3 = 1.$$
 (3)

The REV of the MgO-C foam can be substituted in a homogenised sense by the concept of volume fractions according to Figure 1 (c). For multiphase materials, two different densities can be defined. The real density $\rho^{\beta R} = dm^{\beta}/dv^{\beta}$ is the local quotient of the local mass element dm^{β} and the local volume element dv^{β} . Whereas, the partial density $\rho^{\beta} = dm^{\beta}/dv$ is the quotient of the local mass element dm^{β} and the volume element of the mixture dv. Both densities are coupled by the volume fraction

$$\rho^{\beta} = n^{\beta} \rho^{\beta R}. \tag{4}$$

It is assumed, that the two solid phases (phase (1), C and phase (2), MgO) of the cellular refractories are materially incompressible but due to the compressibility of the pore phase (phase (3), air), they possess a structural compressibility in the macro model. This leads to the geometrical constraint, that the real densities $\rho^{\beta R}$ of the solid phases

are constant. Due to the compressibility of the pore gas, the mixture is also compressible. Carbon and MgO have a changing partial density ρ^{β} , since the volume fractions n^{β} and hence the partial densities change with compression of the mixture. The total volume reduces by compression, the pore volume vanishs at the point of compaction, but the solid body mass m^{β} stays constant. As a result, the partial density ρ^{β} increases.

$$\rho^{\beta R} = \text{const.} \quad \beta = 1, 2 \quad \text{and} \qquad \rho^{\beta} = \frac{\mathrm{d}m^{\beta}}{\mathrm{d}v} \neq \text{const.}$$
(5)

The TPM combines the theory of mixture with the concept of volume fractions and assumes that all constituents are statistically distributed in the REV leading to a statistic substitute model for the mixture with superimposed and interacting constituents [5]. The spatial point \mathbf{x} of the current configuration is at the same time occupied by material points of all constituents φ^{β} . Material points of individual constituents follow their own motion function χ_{β} and hence, originate from different initial positions \mathbf{X}^{β} .

In contrast to the TPM, in our multiphase approach of porous media, it is assumed, that individual phases do not interpenetrate. In these modified superimposed continua for MgO-C foams, material points of the three phases (C, MgO, air) originate from the same initial position \mathbf{X} , follow the same motion function $\boldsymbol{\chi}$ and occupy the same point \mathbf{x} at the time t (see Figure 2).

$$\mathbf{x} = \boldsymbol{\chi}_{\boldsymbol{\beta}} \left(\mathbf{X}_{\boldsymbol{\beta}}, t \right) = \boldsymbol{\chi} \left(\mathbf{X}, t \right) \qquad \forall \boldsymbol{\beta}$$
(6)

with
$$\mathbf{X}_{\beta} = \boldsymbol{\chi}_{\boldsymbol{\beta}} (\mathbf{X}_{\beta}, t_0) = \boldsymbol{\chi} (\mathbf{X}, t_0) = \mathbf{X} = \boldsymbol{\chi}^{-1} (\mathbf{x}, t)$$
 (7)

For the velocity refered to the reference configuration, one has

$$\mathbf{v}_{\beta}\left(\mathbf{X}_{\beta},t\right) = \frac{\partial \boldsymbol{\chi}_{\beta}\left(\mathbf{X}_{\beta},t\right)}{\partial t} = \frac{\partial \boldsymbol{\chi}\left(\mathbf{X},t\right)}{\partial t}$$
(8)

And with respect to the current configuration, one obtains

$$\mathbf{v}_{\beta}\left(\mathbf{x},t\right) = \mathbf{x}_{\beta}'\left(\boldsymbol{\chi}_{\beta}^{-1}\left(\mathbf{x},t\right),t\right) = \mathbf{x}_{\beta}'\left(\mathbf{x},t\right)$$
(9)

As a result, the velocities \mathbf{v}_{β} of all constituents are equal $\mathbf{v} = \mathbf{v}_{\beta} = \mathbf{v}_1 = \mathbf{v}_2 = \mathbf{v}_3$. The deformation gradient \mathbf{F}_{β} with respect to a motion $\boldsymbol{\chi}_{\beta}$ of a constituent φ^{β} is

$$\mathbf{F}_{\beta} = \frac{\partial \boldsymbol{\chi}_{\beta} \left(\mathbf{X}_{\beta}, t \right)}{\partial \mathbf{X}_{\beta}} = \operatorname{Grad}_{\beta} \boldsymbol{\chi}_{\beta} = \operatorname{Grad}_{\mathbf{X}} = \mathbf{F}.$$
 (10)

According to the assumption that the motion functions of all constituents φ^{β} are equal, the deformation gradient and the Jacobi determinant of all phases are equal, as well.

$$\mathbf{F} = \mathbf{F}_{\beta}$$
 and $J_{\beta} = \det \mathbf{F}_{\beta} = \det \mathbf{F}$ with $\beta = 1, 2, 3$ (11)



Figure 2: Kinematics for the modified superimposed continua of MgO-C foams

3 BALANCE EQUATIONS FOR MgO-C FOAMS

Balance equations for mixtures can be deduced from Truesdells three methaphysic principes [3]. All properties of the mixture must be mathematical consequences of the properties of all constituents. To describe the motion of one constituent, conceptually, one can separate this constituent from the residual constituents of the mixture, on condition that the influence of the other constituents is considered. By the introduction of the production terms in the balance equations, the interaction between the constituents φ_{β} can be described. And finally, the motion of the mixture is governed by the same equations as the motion of an one-phase material. The general local form of balance equations for one phase materials is [5]

$$\dot{\psi}_{\beta} + \psi \operatorname{div} \dot{\mathbf{x}} = \operatorname{div} \phi + \sigma + \hat{\psi}$$
 (12)

with ()[•] representing the total time derivative with respect to the baroccentric velocity. Hence, the local form of the balance equations for the various constituents φ^{β} is

$$\left(\boldsymbol{\psi}_{\boldsymbol{\beta}}\right)_{\boldsymbol{\beta}}' + \boldsymbol{\psi}_{\boldsymbol{\beta}} \operatorname{div} \mathbf{x}_{\boldsymbol{\beta}}' = \operatorname{div} \boldsymbol{\phi}_{\boldsymbol{\beta}} + \boldsymbol{\sigma}_{\boldsymbol{\beta}} + \hat{\boldsymbol{\psi}}_{\boldsymbol{\beta}}, \tag{13}$$

whereas $(\cdot)_{\beta}$ is the material time derivative, which describes the changes of Ψ that an observer experienced who moved with the material point \mathbf{X}_{β} .

Before deducing the individual balance equations for the mixture and the various constituents, there is a short summary of all assumptions made up to now and further assumptions for the evaluation of the balance equations.

- [A1] Concept of volume fractions and superimposed continua
- [A 2] Material <u>in</u>compressibility but structural compressibility for phase (1), C & (2), MgO
- [A 3] Material compressibility for phase (3), the pore fluid, air
- [A 4] Superimposed continua with equal motion functions $\chi_{meta}=\chi$

- [A 5] For each point in time, the constituents occupy the same place
- [A 6] Truesdells metaphysical principle
- [A7] No mass exchange between the various constituents

3.1 Mass balances

The local form of the mass balance of the mixture is

 $\dot{\rho} + \rho \operatorname{div} \dot{\mathbf{x}} = 0$ yielding $\rho = \rho_0 \operatorname{det} \mathbf{F}^{-1}$ with ρ_0 : reference density (14)

Because of the fact, that the pore fluid is compressible, the mixture is compressible as well, although the phase (1) and phase (2) are incompressible.

The partial mass balances for each phase φ^{β} deduce by the extension of the axiom of mass conservation by production terms. In general, the mass of one constituent stays not constant, it changes by mass exchange between the various constituents of the mixture, e. g. by melting of ice or chemical reactions.

$$(\rho^{\beta})'_{\beta} + \rho^{\beta} \operatorname{div} \mathbf{v}_{\beta} = \hat{\rho}^{\beta} \quad \text{with} \quad \mathbf{v}_{\beta} = \mathbf{x}'_{\beta}$$
 (15)

With assumption [A 4] of equal motion functions and [A 7], no mass exchange between the various constituents, the mass balance for the various constituents φ^{β} becomes to

$$\left(\rho^{\beta}\right)_{\beta}' + \rho^{\beta} \operatorname{div} \mathbf{v}_{\beta} = 0 \quad \text{with} \quad \rho^{\beta} = n^{\beta} \rho^{\beta R}$$
 (16)

$$\Rightarrow n^{\beta} \left(\rho^{\beta R}\right)_{\beta}' + \rho^{\beta R} \left(n^{\beta}\right)_{\beta}' + n^{\beta} \rho^{\beta R} \operatorname{div} \mathbf{v}_{\beta} = 0$$
(17)

For the three phases, different assumptions concerning the compressibility were taken, leading to different mass balances. Phase (1), C and (2) MgO are material <u>in</u>compressible, hence, the mass balance reduces to a volume balance

$$\left(\rho^{\beta R}\right)_{\beta}' = 0 \quad \Rightarrow \quad \left(n^{\beta}\right)_{\beta}' + n^{\beta} \operatorname{div} \mathbf{v}_{\beta} = 0 \quad \text{for} \quad \beta = 1, 2$$
 (18)

Since all velocities of the phases are equal, the material time derivative is equal to the total time derivative $(n^{\beta})'_{\beta} = \dot{n}^{\beta}$ and it follows directly by integration of Eq. 18

$$n^{\beta} = n_0^{\beta} \det \mathbf{F}_{\beta}^{-1} = n_0^{\beta} \det \mathbf{F}^{-1}$$
(19)

In contrast to the carbon and magnesia phase, phase (3), the pore gas is materially compressible. In the mass balance of Eq. (17), n^{β} will be replaced by $n^3 = 1 - n^1 - n^2$ according to the saturation condition (Eq. (3)). The material time derivative $(n^3)'_3$ can be replaced using the definition of the material time derivative and the volume balance for phase (1) and (2) (Eq. (18)) by

$$(n^3)'_3 = n^1 \operatorname{div} \mathbf{v_1} - \operatorname{grad} (n^1) (\mathbf{v_3} - \mathbf{v_1}) + n^2 \operatorname{div} \mathbf{v_2} - \operatorname{grad} (n^2) (\mathbf{v_3} - \mathbf{v_2})$$
(20)

Based on assumption [A 4] with equal motion functions, the velocities are equal, as well $\mathbf{v} = \mathbf{v_1} = \mathbf{v_2} = \mathbf{v_3}$. Hence, there is no relative velocity between the various phases and the seepage velocity between the phases became zero, whereas all diffusion terms and gradients vanish. The material time derivative reduces to

$$(n^3)'_3 = (n^1 + n^2) \operatorname{div} \mathbf{v}.$$
 (21)

Hence, the mass balance of the pore gas reduces to

$$(1 - n^{1} - n^{2}) (\rho^{3R})'_{3} + \rho^{3R} \operatorname{div} \mathbf{v} = 0.$$
(22)

With div $\mathbf{v} = (\det \mathbf{F})^{\bullet} / \det \mathbf{F}$ and $n^{\beta} = n_0^{\beta} \det \mathbf{F}^{-1}$ the mass balance for the compressible pore gas follows by direct integration

$$\rho^{3R} = \rho_0^{3R} \frac{1 - n_0^1 - n_0^2}{\det \mathbf{F} - n_0^1 - n_0^2}$$
(23)

3.2 Momentum balance

The change of the momentum of a body is caused by any force acting on the body. Disregarding external forces, for the momentum balance of the mixture, one has

$$\rho \ddot{\mathbf{x}} = \operatorname{div} \mathbf{T} + \mathbf{b} \tag{24}$$

The partial momentum balance of the constituent φ^{β} with the partial stress \mathbf{T}^{β} is

$$\rho^{\beta} \mathbf{x}_{\beta}^{\prime\prime} = \operatorname{div} \mathbf{T}^{\beta} + \mathbf{b}^{\beta} + \hat{\mathbf{p}}^{\beta}$$
(25)

The momentum production term $\hat{\mathbf{p}}^{\beta}$ describes the interaction forces between the various constituents φ^{β} . The stress tensor of the mixture consists of the sum of the partial stresses and the diffusion terms, where \mathbf{x}'_{β} is the velocity of the constituent φ_{β} and \mathbf{d}_{β} is the relative motion by the diffusion velocity

$$\mathbf{T} = \sum_{\beta} \left(\mathbf{T}^{\beta} - \rho^{\beta} \mathbf{x}_{\beta}^{\prime} \otimes \mathbf{d}_{\beta} \right) \quad \text{with } [\mathbf{A} \, 4] \quad \Rightarrow \quad \mathbf{T} = \sum_{\beta} \mathbf{T}^{\beta} \tag{26}$$

With assumption [A 4], there is no relative motion between the various phases, whereas the diffusion part $\rho^{\beta} \mathbf{x}_{\beta}' \otimes \mathbf{d}_{\beta}$ is zero. The stress tensor of the mixture is the sum of the stresses of its constituents. The constituents are allowed to exchange momentum, but a production of momentum for the whole mixture is not acceptable, hence $\sum_{\beta} \hat{\mathbf{p}}^{\beta} = \mathbf{0}$.

4 LINEAR THERMOELASTICITY FOR MgO-C FOAMS

4.1 Strain measures by multiplicative decomposition of F

For the evaluation of strain measures of the phases (1), C and (2), MgO, the deformation gradient **F** will be multiplicatively decomposed, according to Figure 3. The intermediate configuration \mathcal{B}_{θ} at a nonuniform temperature θ is obtained from the deformed



Figure 3: Multiplicative decomposition of the deformation gradient **F** in a thermal $\mathbf{F}^{\beta,\theta}$ and an elastic part $\mathbf{F}^{\beta,el}$ for the constituent φ^{β} ; $\mathbf{F} = \mathbf{F}^{\beta} = \mathbf{F}^{\beta,el} \cdot \mathbf{F}^{\beta,\theta}$.

configuration \mathcal{B} by isothermal destressing to zero stress. The deformation gradient from initial to deformed configuration \mathbf{F} is decomposed into an elastic part \mathbf{F}^{el} and a thermal part \mathbf{F}^{θ} , such that $\mathbf{F} = \mathbf{F}^{\theta} \cdot \mathbf{F}^{el}$ [6, 7]. Under the assumption of equal motion functions [A4] it follows that

$$\mathbf{F} = \mathbf{F}^{\beta} = \mathbf{F}^{\beta,\theta} \cdot \mathbf{F}^{\beta,el} \tag{27}$$

Where $\mathbf{F}^{\beta,\theta}$ describes the thermal deformation and $\mathbf{F}^{\beta,el}$ the elastic deformation of the constituent φ^{β} . Under the assumption of isotropy and pure volumetric temperature evolution, $\mathbf{F}^{\beta,\theta} \cdot \mathbf{F}^{\beta,el}$ leads to the same result as $\mathbf{F}^{\beta,el} \cdot \mathbf{F}^{\beta,\theta}$ [6]. For the thermal part of the deformation gradient under the above-mentioned assumptions, one has

$$\mathbf{F}^{\beta,\theta} = \vartheta_{\beta}(\theta) \,\mathbf{I} \tag{28}$$

where $\vartheta_{\beta}(\theta)$ is the thermal stretch ratio. With the linear coefficient of thermal expansion (CTE) α , the thermal stretch ratio can be written as

$$\vartheta_{\beta}(\theta) = \frac{l}{l_0} = 1 + \alpha(\theta) \,\Delta T \approx 1 + \alpha_0 \left(\theta - \theta_0\right) \tag{29}$$

 ΔT describes the temperatue difference between the temperature θ_0 in the reference configuration and the temperature θ of the thermal intermediate configuration. Based on the different CTEs of carbon and magnesia ($\alpha_C \neq \alpha_{MgO}$), the thermal part of the deformation gradient differs for each phase, whereas the total deformation gradient is equal. For the Green-Lagrangian strain tensor, reads as follows

$$\mathbf{E} = \frac{1}{2} \left(\mathbf{F}^{\mathbf{T}} \cdot \mathbf{F} - \mathbf{I} \right) = \mathbf{E}^{\beta} = \frac{1}{2} \left((\mathbf{F}^{\beta})^{\mathbf{T}} \cdot \mathbf{F}^{\beta} - \mathbf{I} \right)$$
(30)

The thermal strain of the mixture on the reference configuration is defined by

$$\mathbf{E}^{\theta} = \frac{1}{2} \left((\mathbf{F}^{\theta})^T \cdot \mathbf{F}^{\theta} - \mathbf{I} \right)$$
(31)

The thermal strains of the various constituents are defined by

$$\mathbf{E}^{\beta,\theta} = \frac{1}{2} \left((\mathbf{F}^{\beta,\theta})^T \cdot \mathbf{F}^{\beta,\theta} - \mathbf{I} \right)$$
(32)

The Green-Lagrangian strain can be additively splitted into

$$\mathbf{E} = \mathbf{E}^{\theta} + \mathbf{E}^{el} \tag{33}$$

The elastic Lagrangian strain $\mathbf{E}^{el} = \mathbf{E} - \mathbf{E}^{\theta}$ defined relative to \mathcal{B} is a mixed term of \mathbf{E}^{el} and \mathbf{E}^{θ} . With the push-forward operation, the Lagrangian strain $\hat{\boldsymbol{\Gamma}}^{el}$ relative to the intermediate configuration \mathcal{B}_{θ} at non-uniform temperature θ relates to

$$\hat{\boldsymbol{\Gamma}}^{el} = (\mathbf{F}^{\theta})^{-T} \left(\mathbf{E} - \mathbf{E}^{\theta} \right) (\mathbf{F}^{\theta})^{-1} = \frac{1}{\vartheta^2} \left(\mathbf{E} - \mathbf{E}^{\theta} \right)$$
(34)

Using Eq. 28 and the symmetry of the thermal deformation gradient, the thermal strain in Eq. 31 becomes to

$$\mathbf{E}^{\theta} = \frac{1}{2} \left(\vartheta^2 - 1 \right) \mathbf{I}$$
(35)

By substituting \mathbf{E}^{θ} in equation Eq. 34 in relation to \mathcal{B}_{θ} , the elastic strain on the intermediate configuration can be expressed by the total Lagrangian strain \mathbf{E} of the reference configuration and the thermal stretch ratio ϑ as

$$\hat{\boldsymbol{\Gamma}}^{el} = \frac{1}{2} \left(\frac{1}{\vartheta^2} - 1 \right) \mathbf{I} + \frac{1}{\vartheta^2} \mathbf{E}.$$
(36)

Since the overall strains **E** for all phases are equal (see Eq. 30), the elastic strain for each phase is distinguished by the thermal stretch ratio ϑ_{β} and hence, by the linear coefficient of thermal expansion α_{β} . The elastic strain for the constituent φ^{β} becomes to

$$\hat{\boldsymbol{\Gamma}}^{el,\beta} = \frac{1}{2} \left(\frac{1}{\vartheta_{\beta}^2} - 1 \right) \mathbf{I} + \frac{1}{\vartheta_{\beta}^2} \mathbf{E}.$$
(37)

4.2 Stresses based on linear thermoelasticity

Using the concept of multiplicative decomposition of the deformation by the introduction of a thermal intermediate configuration, the Helmholtz free energy for the various constituents φ^{β} can be additively split into an isotropic function $\psi^{el,\beta}$ of the elastic strain $\hat{\Gamma}^{el,\beta}$ and the temperature θ and a part $\psi^{\theta,\beta}$ only dependent on the temperature, according to [7]

$$\psi^{\beta} = \psi^{el,\beta} \left(\hat{\Gamma}^{el,\beta}, \theta \right) + \psi^{\theta,\beta}$$
(38)

The partial stress \mathbf{T}^{β} relies only on the elastic strains and the elastic part of the free energy, but it is weighted by the thermal stretch ratio [7],

$$\mathbf{T}^{\beta} = \frac{\rho_{\beta,0}}{\vartheta_{\beta}^2} \frac{\partial \psi^{el,\beta}}{\partial \hat{\mathbf{\Gamma}}^{el,\beta}} \tag{39}$$

With the relationship $\rho_{\beta,0} = \vartheta_{\beta}^3 \rho_{\beta,\theta}$, between the densities $\rho_{\beta,0}$ of the reference configuration and $\rho_{\beta,\theta}$ in the intermediate configuration, the stress response can also be written as

$$\mathbf{T}^{\beta} = \vartheta_{\beta} \mathbf{T}^{el,\beta}, \qquad \mathbf{T}^{el,\beta} = \rho_{\beta,0} \frac{\partial \psi^{el,\beta}}{\partial \hat{\Gamma}^{el,\beta}}$$
(40)

For the suggestion, that the Helmholtz free energy $\psi^{el,\beta}$ is a quadratic function of the elastic strain components, such that

$$\rho_{\beta,\theta} \psi^{el,\beta} = \frac{1}{2} \lambda_{\beta}(\theta) \left(\operatorname{tr} \left(\hat{\boldsymbol{\Gamma}}^{el,\beta} \right) \right)^2 + \mu_{\beta}(\theta) \, \hat{\boldsymbol{\Gamma}}^{el,\beta} : \hat{\boldsymbol{\Gamma}}^{el,\beta}$$
(41)

whereas $\lambda_{\beta}(\theta)$ and $\mu_{\beta}(\theta)$ are the temperature-dependent Lamé constants of the various solid phases φ^{β} . It follows, that

$$\mathbf{T}^{el,\beta} = \mathbb{C}^{el,\beta}(\theta) : \hat{\mathbf{\Gamma}}^{el,\beta}, \quad \text{with} \quad \mathbb{C}^{el,\beta}(\theta) = \lambda_{\beta}(\theta) \mathbf{I} \otimes \mathbf{I} + 2\,\mu_{\beta}(\theta) \,\mathbb{I}$$
(42)

Where \mathbb{I} is the fourth-oder unit tensor

$$\mathbb{I}_{ijkl} = \frac{1}{2} \left(\delta_{ik} \, \delta_{jl} + \delta_{il} \, \delta_{jk} \right) \tag{43}$$

According to the assumptions for the motion function [A 4] and the deformation gradient of the various constituents, the overall strain of the mixture is equal to the partial overall strains, $\mathbf{E} = \mathbf{E}^{\beta} = \mathbf{E}^{1} = \mathbf{E}^{2}$ since $\mathbf{F} = \mathbf{F}^{\beta} = \mathbf{F}^{1} = \mathbf{F}^{2}$. By substituting Eq. 42 and Eq. 36 into Eq. 40, based on the isotropic linear thermoelasticity, the partial stress \mathbf{T}^{β} for the various constituents φ^{β} is

$$\mathbf{T}^{\beta} = \frac{1}{\vartheta_{\beta}} \left[\lambda_{\beta}(\theta) \operatorname{tr}(\mathbf{E}) \mathbf{I} + 2\,\mu_{\beta}(\theta) \,\mathbf{E} \right] + \frac{1}{2} \mathbf{I} \left(\frac{1}{\vartheta_{\beta}} - \vartheta_{\beta} \right) \left[3\,\lambda_{\beta}(\theta) + 2\,\mu_{\beta}(\theta) \right]$$
(44)

Notice, the thermal stretch ratio $\vartheta_{\beta}(\theta)$ depends also on the temperature. Replacing the Lamé constant λ_{β} by the compression modulus κ_{β} with

$$\kappa_{\beta}(\theta) = \lambda_{\beta} + \frac{2\mu_{\beta}}{3} \iff \lambda_{\beta} = \kappa_{\beta} - \frac{2\mu_{\beta}}{3}$$
(45)

the partial stress can be written as

$$\mathbf{T}^{\beta} = \frac{1}{\vartheta_{\beta}(\theta)} \left[\lambda_{\beta}(\theta) \operatorname{tr}(\mathbf{E}) \mathbf{I} + 2\,\mu_{\beta}(\theta) \,\mathbf{E} \right] + \frac{3}{2} \left(\frac{1}{\vartheta_{\beta}(\theta)} - \vartheta_{\beta}(\theta) \right) \,\kappa_{\beta}(\theta) \,\mathbf{I}$$
(46)

If the Lamé constants are taken to be temperature-independent, and if for the thermal stretch ratio, the approximation $\vartheta_{\beta}(\theta) \approx 1 + \alpha_{\beta,0} (\theta - \theta_0)$ is used, the partial Cauchy stress \mathbf{T}^{β} can be expressed by the infinitesimal strain \mathbf{E} in form of the *Duhamel-Neumann* expression of isotropic linear thermoelasticity [8, 9].

$$\mathbf{T}^{\beta} = \lambda_{\beta,0} \operatorname{tr}(\mathbf{E}) \mathbf{I} + 2 \,\mu_{\beta,0} \mathbf{E} - 3 \,\alpha_{\beta,0} \left(\theta - \theta_{\beta,0}\right) \,\kappa_{\beta,0} \mathbf{I}$$
(47)

Hence, the partial stresses of the phases (1), C and (2), MgO depend on the same strain **E** but differ according to the different Lamé constants and CTEs.

5 CONSTITUTIVE EQUATIONS FOR MgO-C FOAMS

The constitutive equation for the MgO-C foams is evaluated using the rule of mixture for the partial stresses \mathbf{T}^{β} , whereas the partial stresses are weighted by their volume fraction n^{β} . The pore pressure p^3 is caused by the compression of the mixture, leading to the compression of the pore gas (phase (3), air). According to Newton's law 'actio = reactio', the pore pressure p^3 acts on the both other phases and hence contributes to 100% to the stress of the mixture. For the overall stress of the MgO-C foams, made of the three phases, one has

$$\mathbf{T} = -p^3 \mathbf{I} + n^1 \mathbf{T}^1 + n^2 \mathbf{T}^2$$

$$\tag{48}$$

To describe the evaluation of the pore pressure p under deformation of the mixture, the ideal gas law was used as equation of state for the pore gas.

$$pV = nR\theta$$
 with $\rho = \frac{m}{V}$ and $M = \frac{m}{n}$ (49)

V denotes to the gas volume, n is the amount of substance, R the ideal gas constant, m the mass and M the molar mass of the gas. Finally, using the mass balance for the pore gas (Eq. 23), the pore pressure p^3 can be determined by

$$p^{3} = \rho_{0}^{3R} \frac{R\theta}{M^{air}} \frac{1 - n_{0}^{1} - n_{0}^{2}}{\det \mathbf{F} - n_{0}^{1} - n_{0}^{2}}$$
(50)

6 CONCLUSIONS

In this contribution, we presented a new multiphysics approach for porous media, especially cellular MgO-C refractories. The key assumption is the use of the theory of porous media (TPM) with a kinematic coupling of the displacement and temperature fields of all constituents. It was assumed, that there is no interdiffusion of the three constituents (MgO, C and pore gas) with the result that the motion functions and hence the deformation gradients of all phases are equal. Linear thermoelasticity with a multiplicative decomposition of the deformation gradient into an elastic and a thermal part for isotropic materials according to the Duhamel-Neumann relation was extended to the mixture of MgO and C phase. The difference in the coefficient of thermal expansion (CTE) leads to different thermal induced stresses in both phases. For the pore gas, the ideal gas law was used as equation of state for the evolution of pressure as function of the density and the temperature. The total macroscopic stress was calculated using the theory of mixture, inclusing the contributions from the pore pressure and the two solid phases.

REFERENCES

- [1] Falk G, Jung A, Da Silveira W, Diebels S. Experimental characterization and thermo-mechanical modelling of micro structure interactions in cellular carbon magnesia refractories. J. Ceram. Sci. Tech. (2014) 5(2):101–114.
- [2] Jung A, Falk G, Petri D, Diebels S. Thermal shock resistivity of hybrid carbon foam materials: Experiments and model predictions. *Mech. Mater.* DOI: 10.1016/j.mechmat.2014.12.007
- [3] Truesdell, C. and Toupin, A. The classical field theories. Handbuch der Physik, Band III/1, Springer-Verlag, (1960).
- [4] Bowen, R. M. Incompressible porous media models by use of the theory of mixtures. Int. J. Engng. Sci. (1980) 18:1129–1148.
- [5] Ehlers, W. Grundlegende Konzepte in der Theorie Poröser Medien. Tech. Mech. (1996) 16:63–76.
- [6] Hartmann, S. Comparison of the multiplicative decomposition $F=F_{\theta}F_{M}$ and $F=F_{M}F_{\theta}$ in finite strain thermoelasticity. *Technical Report Series TU Clausthal, Clausthal University of Technology* (2001):Fac3-12-01.
- [7] Lubarda, V.A. Constitutive theories based on the multiplicative decomposition of deformation gradient: Thermoelasticity, elastoplasticity, and bimechanics. *Appl. Mech. Rev.* (2004) 57(2):95–108.
- [8] Carlson, D.E. Linear thermoelasticity, Handbuch der Physik, Band VIa/2. Springer-Verlag, (1972).
- [9] Nowacki, W. Thermoelasticity. Pergamon Press, (1986).