8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineeering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

Thermomechanical Energetic Models for Multi-phase Materials

*** T.-A. Langhoff, T. Böhlke and E. Schnack**

Institut für Technische Mechanik, Universität Karlsruhe (TH)
Universität Karlsruhe (TH), Postfach 6980, 76128 Karlsruhe, Germany
langhoff@itm.uni-karlsruhe.de, boehlke@itm.uni-karlsruhe.de
eckart.schnack@imf.mach.uka.de, www.itm.uni-karlsruhe.de

Key Words: *Energetic model, Dissipation, Thermoelasticity, Convex potentials*

ABSTRACT

In an isothermal framework, energetic models based on the works of MIELKE [1] have been meanwhile established for very different situations, e.g. shape memory alloys [2], crack growth [3], etc.. They are also applicable in case of non-convex potentials of multi-phase materials [4]. The main ingredients are the stored energy functional $\mathcal{E}$, that depends on the admissible displacement field $\boldsymbol{u}$ and the phase distribution $\boldsymbol{s}$ within the domain $\Omega \subset \mathbb{R}^d$, and the dissipation functional $\mathcal{D}$ giving the dissipated energy in case of phase transformations (i.e. a change of the phase distribution within Ω). Both functionals $\mathcal{E}$ and $\mathcal{D}$ occur in a static stability inequality and in an energy conservation equation in the following energetic formulation: Find among all admissible displacement fields $\tilde{\boldsymbol{u}}$ and phase distributions $\tilde{\boldsymbol{s}}$ the solution $(\boldsymbol{u}, \boldsymbol{s})$ such that

$$\mathcal{E}(t, \boldsymbol{u}, \boldsymbol{s}) \leq \mathcal{E}\left(t, \tilde{\boldsymbol{u}}, \tilde{\boldsymbol{s}}\right) + \mathcal{D}\left(\boldsymbol{s}(t), \tilde{\boldsymbol{s}}\right) \tag{1}$$

and

$$\mathcal{E}(t, \boldsymbol{u}, \boldsymbol{s}) + \mathcal{E}_{diss}(t, \boldsymbol{s}) = \mathcal{E}\left(0, \boldsymbol{u}_0, \boldsymbol{s}_0\right) - \tilde{\mathcal{E}}_{ext}(t, \boldsymbol{u})\,, \tag{2}$$

where $\tilde{\mathcal{E}}_{ext}$ denotes the energy due to external load and $\mathcal{E}_{diss}(t, \boldsymbol{s})$ is the complete dissipated energy up to time t. A time incremental formulation of (1) and (2) yields an infimum problem for a partition $\{t_k\}$ of the given time interval

$$\mathcal{E}\left(t_k, \boldsymbol{u}_k, \boldsymbol{s}_k\right) = \inf_{(\boldsymbol{u}, \boldsymbol{s})} \left\{\mathcal{E}\left(t_k, \boldsymbol{u}, \boldsymbol{s}\right) + \mathcal{D}\left(\boldsymbol{s}_{k-1}, \boldsymbol{s}\right)\right\} \tag{3}$$

From theoretical point of view, the main advantage is that energetic models admit solutions under weak regularity requirements. Additionally, convexity assumptions can be replaced by requirements on the external loading.

Actually, for applying such theories thermal dependencies have to be included since many composites and multi-phase materials are either produced by or designed to withstand thermal-mechanical loading. Thus, a thermomechanical extension of the isothermal energetic models is needed. First existence results for non-isothermal energetic models have been obtained [5] assuming a known equilibrium solution of the thermal problem.

As an extension of [5] we propose a thermo-mechanical microscopic energetic model [6]. The consideration of thermal effects results in a twofold coupling: on the one hand, the coupled nature of thermo-elasticity itself is respected, and on the other hand temperature dependent phase transformations within the material directly influence the dissipation functional $\mathcal{D}$ as well as the energy functional $\mathcal{E}$. Thus in (1) and (2) the temperature θ has to be considered as an additional independent variable. Moreover, a new thermal contribution W_{th} to the stored energy density W emerges

$$W_{th}(\boldsymbol{x}, \boldsymbol{Du}, \boldsymbol{s}, \theta) = \int_{\theta_0}^{\theta} \sum_{p\in\mathcal{P}} \mathbf{1}_{\Omega_p}(\boldsymbol{x})\, c^{(p)}(\theta')\, \mathrm{d}\theta' + \sum_{p\in\mathcal{P}} \mathbf{1}_{\Omega_p}(\boldsymbol{x})\, \boldsymbol{b}^{(p)} : (\boldsymbol{Du})\ (\theta - \theta_0) \tag{4}$$

where $\mathcal{P}$ denotes the set of phases within the material, $\Omega_p \subset \Omega$ the domain occupied by the phase $p \in \mathcal{P}$, $c^{(p')}(\theta)$ the temperature-dependent specific heat of the different phases and $\boldsymbol{b}$ denotes a tensor of second order as the generalization of the linear thermal expansion coefficient in case of anisotropic material behaviour. Restrictions on the energy contributions and the material parameters in combination with convexity requirements are studied to guarantee the existence of solutions. Under suitable conditions, a new strongly staggered scheme is defined for a first numerical solution procedure of the coupled thermo-mechanical energetic model [7].

An application besides shape memory alloys is to model the thermo-mechanical response of carbon fibre reinforced carbon where the microstructure is temperature-dependently formed by different textures of pyrolytic carbon [8].

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