Special Session 33: Thermomechanics and Phase Change

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Free boundary problems for a valve mede of shape memory alloys

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In this talk we consider a free boundary problem describing a change of the length of a one-dimensional elastic material. By elementary calculation the free boundary problem is given as the initial boundary value problem for the hyperbolic equation with dynamic boundary condition. Moreover, as the practical example for the elastic material we deal with a new mathematical model for a valve made of a shape memory alloy spring and a normal spring. The model is given by the following initial boundary value problem:

$$
\begin{aligned}
&\rho_1 u_{1tt} + \gamma u_{1xxxx} - (\theta u_{1x} + f(u_{1x}))_x = \rho_1 g_1 \\
&\qquad\qquad\qquad\qquad \text{in } Q_1(T),\\
&\rho_2 u_{2tt} - \kappa u_{2xx} = \rho_2 g_2 \\
&\qquad\qquad\qquad\qquad \text{in } Q_2(T),\\
&m\ell''(t) = mg_3 - (\theta u_{1x})(t, L_1-) + \kappa u_{2x}(t, L_1+) \\
&\qquad\qquad + \gamma u_{1xxx}(t, L_1-) \\
&\qquad\qquad\qquad\qquad \text{for } 0 < t < T,\\
&u_1(t,0) = 0, u_2(t,L) = 0, u_{1xx}(t,0) = u_{2xx}(t,L_1) = 0 \\
&\qquad\qquad\qquad\qquad \text{for } 0 < t < T,\\
&u_1(t,L_1) = u_2(t,L_1), \ell(t) = u_1(t,L_1) + L_1 \\
&\qquad\qquad\qquad\qquad \text{for } 0 < t < T,\\
&u_1(0,x) = u_{01}(x), u_{1t}(0,x) = v_{01}(x) \\
&\qquad\qquad\qquad\qquad \text{for } 0 < x < L_1,\\
&u_2(0,x) = u_{02}(x), u_{2t}(0,x) = v_{02}(x) \\
&\qquad\qquad\qquad\qquad \text{for } L_1 < x < L,
\end{aligned}
$$

where ρ_1 (resp. ρ_2) is the density of the shape memory alloy (resp. the normal) spring, γ is a positive constant,θ is the given temperature field, $f : R \to R$ is the free energy function?g_1, g_2 and g_3 are given functions, and u_{01}, v_{01}, u_{02} and v_{02} are initial functions.

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Shape-memory alloys: effective modelling

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The employment of shape memory alloys (SMA) in a large number of engineering applications, among which biomedical applications, has been the motivation for an increasing interest toward a correct and exhaustive modeling of SMA macroscopic behavior in order to construct reliable simulation tools, which can be successfully used in the design procedures of SMA devices.

In this work we review a robust approach for the development of SMA models, giving a good overall description of pseudo-elastic and shape memory behaviors. We focus on recent model extensions to make the modelling more flexible and reliable in terms of material simulation.

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Investigating adhesive contact by phase transitions

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We introduce a model describing a contact problem with adhesion between a body Ω and a rigid support. It mainly combines damage and contact theories by use of a phase field approach. The PDE system is recovered, in accordance to the theory proposed by Fremond, by thermo-mechanical laws and convex functionals, accounting for possibly physical constraints on the variables of the system. We chose as state variables small deformations in the body described by the strain tensor ε, the temperature of the body θ, the temperature on the contact surface θ_s (which is a priori different from the temperature θ), and a phase parameter χ describing the state of the adhesion on the contact surface. The resulting equations, written both in the body and on the contact surface, are highly nonlinear, mainly for the presence of nonlinear operators (possibly degenerating) accounting for the physical constraints (as the impenetrability condition, the positivity of the absolute temperatures, consistency of the phase parameter). We prove a global in time existence result for the complete system and we investigate the asymptotic behaviour of solutions (characterizing the ω-limit set). In the isothermal case, if the damage process for adhesive bonds is reversible, we also prove uniqueness of the solution and continuous dependence on the data.

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Phase Field Equations: The Next Generation

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After a review of phase field equations and the distinguished sharp interface limits, this talk will focus on new results (obtained in collaboration with Xinfu Chen and Christof Eck). A new derivation from asymptotic analysis leads to a phase field model that is proven to differ by only the square of the interface thickness from the corresponding sharp interface problem. Numerical computations demonstrate the proximity of the diffuse and sharp interface problems using various sets of material parameters including those of succinonitrile experiments on the space shuttle.

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Time-dependent Obstacle problems in thermohydraulics

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Obstacle problems, which are mathematical models of nonlinear phenomena accompanying the free boundary, have been studied. The existence and uniqueness for some systems with the Navier-Stokes equations is considered.

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Phase-field systems with dynamic boundary conditions

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This talk is devoted to the mathematical analyis of a Caginalp type system subject to dynamic boundary conditions which account for possible interactions of the material with the walls enclosing it. We intend to present and discuss a number of recent results about well-posedness, global asymptotic behavior (i.e., attractors) and convergence to single equilibria.

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Phase Transformations in Nanostructures: Models and Applications

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While a phenomenon of phase transformations in infinite nanowires and nanoplates have already been known for some time, the same cannot be said about finite low dimensional nanostructures. Only recently, evidence has been mounting that the phenomenon of phase transformations is important for finite nanostructures too, in particular when predicting opto-electromechanical properties of such structures. Based on our experience with the development of dynamic models for phase transformations at the mesoscopic level [e.g., Comput. Materials Science, 18(3-4), 141-148, 2000; Appl. Numer. Math., 57(5-7), 510-520, 2007], we report here our first attempts to describe phase transformations in finite nano-objects, focusing on the analysis of microstructure evolution. Mathematically, our model is based on a coupled time-dependent system of PDEs and is similar to the model we analyzed in [Heat and Mass Transfer, 43(6), 535-546, 2007]. Several simulation results with this model will be discussed in the context of nanostructures.

Finally, we present several computational results obtained by us with ab initio methodology. We report phase transformations in ZnO and CdS low dimensional nanostructures, including quantum dots, and analyze temperature-dependent phase stability of these objects in the context of their bio-nanotechnological applications.

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Upper bounds for coarsening for the degenerate Cahn-Hilliard equation

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The long time behavior for the degenerate Cahn-Hilliard equation,

$$u_t = \nabla\cdot(1-u^2)\nabla\left[\frac{\Theta}{2}\{\ln(1+u)-\ln(1-u)\}-\alpha u-\epsilon^2\triangle u\right],$$

is characterized by the growth of phase separated domians in which $u \approx u_\pm$, where $u_\pm$ denote the "equilibrium phases;" this process is known as coarsening. The coasening process can be quantified via a characteristic length scale, $l(t)$. Taking $l(t)$ to be prescribed via the Liapunov energy functional and the $(W^{1,\infty})^*$ norm of $u(x,t)$, we prove upper bounds on $l(t)$ for arbitrary mean concentrations, $\bar{u} \in (u_-, u_+)$, and for all temperatures $\Theta \in (0, \Theta_c)$, where Θ_c denotes the "critical temperature." Moreover, we demonstrate that transitions may take place in the nature of the coarsening bounds during the coarsening process. Our results generalize the upper bounds obtained by Kohn & Otto, 2002.

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Global existence for a quasilinear system in thermoviscoelasticity with strain gradient energy

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A three-dimensional thermoviscoelastic system with strain gradient energy (viscosity-capillarity type) describing structural phase transitions in solids is considered. The system, derived from the balance laws of linear momentum and energy, is based on the Landau-Ginzburg free energy functional for the thermal and the total elastic (strain plus strain-gradient) energy. A novel feature of the problem is that the specific heat is not a constant but a function of temperature complying with the third law of thermodynamics. We prove the existence and uniqueness of a regular solution on an arbitrary time interval. The obtained result complements the previous theorem by the authors [SIAM J. Math. Anal. 38, No. 6 (2007), 1733-1759] concerned with the same problem in case of constant specific heat. In the present setup we can admit a stronger thermomechanical coupling. This is a joint work with S. Yoshikawa (Japan) and W. M. Zajączkowski (Poland).

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Bounds on the recoverable strains in composite shape-memory alloys

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New upper bounds are proposed for a generic problem of geometric compatibility, which covers the problem of bounding the effective recoverable strains in composite shape memory alloys (SMAs), such as polycrystalline SMAs or rigidly reinforced SMAs. Both the finite deformation and infinitesimal strain frameworks are considered. The methodology employed is a generalization of a homogenization approach introduced by Milton and Serkov (2000) for nonlinear composites in infinitesimal strains. Some analytical and numerical examples are given to illustrate the method.

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Some results on phase change models with microscopic movements

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This talk will present some recent developments in the analysis of some phase transitions models with microscopic movements proposed by Michel Fre'mond in its monograph [M. Fre'mond: Non-smooth thermomechanics, Springer-Verlag, Berlin (2002)]. The main issue here is to take into account microscopic movements of particles into the description of the phase change phenomenon. It is indeed assumed that this microscopic motion effects are responsible for the phase transition process contributing to the energy balance. The model - which turns out to be consistent with the second principle of thermodynamics - gives rise to a system of strongly nonlinear (and possibly degenerating) PDEs. As a matter of fact we shall note that many classical phase transition model - including, e.g., Stefan problem - can be regarded as a linearization of these models.

This talk will collect some recent contribution in the direction of solving locally or globally in time (some suitable initial-boundary value problem for) the above mentioned PDE systems.

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On the longtime behavior of some variants of the Cahn-Hilliard equation

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In this talk we will present some results on the long time behavior of some variants of the Cahn-Hilliard equation with nonconstant mobility coefficient in three dimensions of space. We will give positive results on the nondegenerate case and partial results on the degenerate case. In the latter case, the presence of a viscosity term will be required. Applications to the thin-film equation will be also discussed. Due to the lack of uniqueness characterizing these problems, the framework of multivalued semiflows will be used in order to study the existence of attractors.

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Uniform attractors for a phase transition model coupling momentum balance and phase dynamics.

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We present some recent result concerning the long time behavior for a mathematical model describing the phase dynamics and the deformations in shape memory alloys. In particular, we discuss about the existence of a uniform attractor.

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Stability analysis for a phase field system associated with linear growth energy

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In this talk, a mathematical model, motivated to represent the dynamics of two-dimensional solid-liquid phase transitions, is considered. The mathematical model is formulated as a system of a heat equation describing the movement of the relative temperature, and an Allen-Cahn type equation which is derived from a free energy containing a convex linear growth function $f \in C(\mathbf{R}^2)$ in the interfacial energy.

The system under consideration is subject to the initial-boundary condition such that the temperature converges to a constant equilibrium state as time goes to infinity. Hence, after a certain large time, the represented physical situations are supposed to be settled some steady-states, that are governed by a single equation associated with the subdifferential of the interfacial energy.

In this talk, the expression of the function f (energy) is restricted to the setting that:

($**$) f forms a Finsler norm, having sublevel sets by regular even-gons (crystalline setting);

to observe, concretely, the anisotropic effects by f to the interfacial patterns in steady-states (steady-state patterns). Consequently, the relationship between the interfacial anisotropy and the stability of the steady-state patterns will be shown from the geometrical viewpoint.

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