

# **Mathematical and Numerical Analysis of Falk-Konopka-type Models for Shape-Memory Alloys**

**Melnik, R.V.N., Roberts, A.J. and Thomas, K.A.**

**Int. Journal of Differential Equations and Applications, 1A(3), 291--300, 2000.**

## **Abstract:**

This paper is devoted to the development of mathematical theory of thermomechanical phase transitions. A hierarchy of mathematical models for smart materials and structures technologies is discussed in the context of models describing shape memory alloy dynamics. The authors analyze mathematical models resulting from the Falk-Konopka generalization of the Landau theory to the meso-scale level. Using center manifold techniques, the authors derive a low-dimensional model obtained directly from the three-dimensional Falk-Konopka model. The results of the theoretical analysis are supported by computational experiments.

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**MATHEMATICAL AND NUMERICAL ANALYSIS  
OF FALK-KONOPKA-TYPE MODELS FOR  
SHAPE-MEMORY-ALLOYS**

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**Abstract:** This paper contributes to the development of mathematical theory of thermomechanical phase transition. We analyse mathematical models resulting from the Falk-Konopka generalisation of the Landau theory to the meso-scale level. Using centre manifold techniques, we derive a low dimensional model obtained directly from the 3D Falk-Konopka model. The results of the theoretical analysis are supported by computational experiments.

**AMS Subj. Classification:** 35M10, 35L70, 65P05, 73F15

**Key Words:** shape memory alloys, low dimensional models, centre manifold reduction.

### **1. Introduction**

One of the major challenges in the development of mathematical theory for smart materials and structures (see Fig. 1) is to adequately describe thermomechanical phase transitions in solids, in particular structural phase transitions between different equilibrium configurations of the metallic lattice of shape-memory alloys (SMA) (see Melnik et al [9]). After being permanently deformed these materials can recover their original shapes upon the change of

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thermo-mechanical conditions. This property, known as the shape-memory effect, has a wide range of applications such as solid-state engines, actuators, work production devices, shape-memory implants, automotive and aerospace applications, vibration control and suppression. The shape memory effect was discovered around 1938 by A. Greninger, V.G. Mooradian, G.V. Kurdumov, but only recently the use of shape-memory materials has become a viable technology and the world-wide business in SMA turned into a sizable industry, growing at over 25% per year.

On the one hand, the development of effective mathematical models and numerical methods for the description of SMA dynamics is required by new applications that ranging from self-erecting devices in aerospace industry to micro-electro-mechanical systems. On the other hand, such applications bring along some of the most challenging problems of modern applied mathematics.

Our starting point in this paper is a system of partial differential equations that includes the equation of motion and the energy balance equation and couples thermal and mechanical fields (see details in Melnik et al [10])

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \cdot \mathbf{s} + \mathbf{F}_1, \quad \rho \frac{\partial e}{\partial t} - \mathbf{s} : (\nabla \mathbf{v}) + \nabla \cdot \mathbf{q} = F_2, \quad (1)$$

where  $e$  is the internal energy,  $\mathbf{s}$  is the stress tensor,  $\rho$  is the density of the material,  $\mathbf{u}$  is the displacement,  $\mathbf{v}$  is the velocity vector,  $\mathbf{q}$  is the heat flux,  $\mathbf{F}_1$ ,  $F_2$  are given forcing functions. We are interested in an adequate mathematical description and computer simulation of the dynamics of shape-memory-alloys in the first-order solid/solid structural phase transitions. This dynamics is a strongly nonlinear phenomenon which is included into system (1) by the constitutive relations,  $\Phi_1(\mathbf{s}, \boldsymbol{\epsilon}) = 0$ ,  $\Phi_2(\mathbf{q}, \theta) = 0$ , that couple stresses, deformation gradients ( $\boldsymbol{\epsilon}$ ), temperature ( $\theta$ ) and heat fluxes.

We organize this paper as follows. In Section 2 we describe main approaches to establish constitutive relations for SMA and discuss a hierarchy of mathematical models applied for modeling of SMA phase transformation. Section 3 is devoted to the Landau-Khalatnikov method that leads to the choice of the free energy function appropriate for the description of phase transitions in SMA materials. A one dimensional hyperbolic approximation of SMA dynamics is given in Section 4, where the methodology for the proof of well-posedness of the problem and our computational schemes are briefly discussed. Finally, Section 5 deals with some key points in low-dimensional modelling of shape-memory-alloy dynamics.

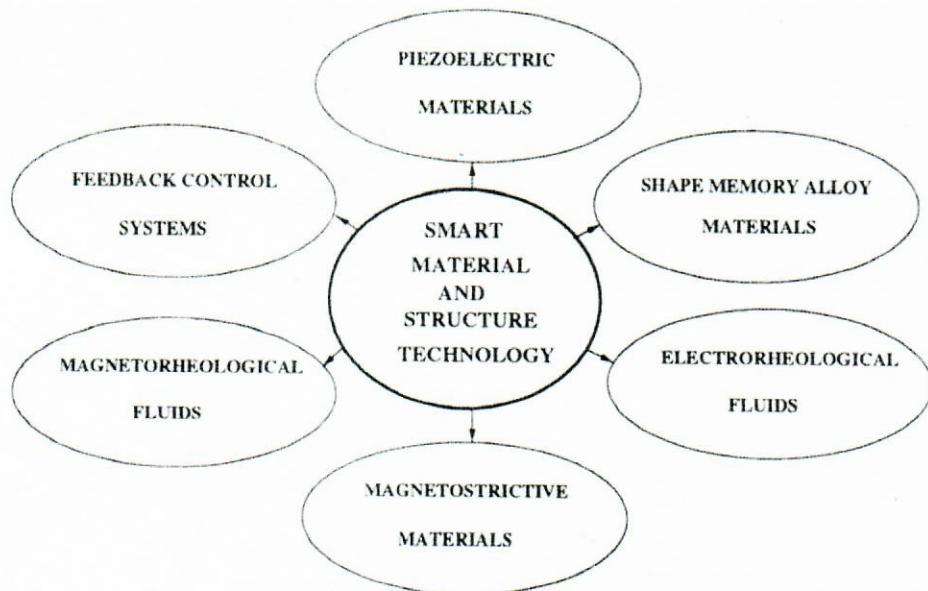


Figure 1: Shape Memory Alloys in Smart Material and Structure Technology

## 2. Hierarchy of Models Describing SMA Dynamics

The dynamics of phase transformations between different equilibrium configurations of the SMA metallic lattice (austenite and martensite) can be described with three different types of mathematical models categorized according to three different spatial length scales: atomic scale, meso-scale and macro-scales. We are interested in austenitic-martensitic crystallographic transformations, i.e. in diffusionless, displacive types solid state transformations, for which no atomic migration is necessary and atoms can cooperatively be rearranged or shifted into a new crystal structure. According to the Landau *microscopic* theory, this atomic shuffling can be examined by using the Bain strain as the basic deformation variable (see Falk [5]). This approach leads to mathematical models with a "hard-to-separate" interdependence of the transformation kinetics and the stress-strain relation. Numerical implementations of such models are limited.

Another method for the construction of mathematical models for SMA material is the *macroscopic* phenomenological method (see Colli [4]). As it was noted by Falk [5] the (macroscopic) deformations in this approach have to be defined at least on a length scale  $100\mu m$ . Although this approach requires a significant amount of experimental work, the resulting mathematical models ignore completely the internal atomic and meso-scale structures of a material.

A reasonable balance between the above extremes can be provided by meso-

scale models which are concerned with the material's internal microstructures, and the shape, size and spatial arrangement of phases. On the mesoscopic scale, it is the shear on the habit plane (the lattice-invariant shear) that acts as the basic deformation variable. Since the spatio-temporal evolution of meso-scale microstructures during solid-solid phase transformations is often an underlying process for the development of many advanced engineering alloys, the construction and investigation of mathematical models at the mesoscopic level constitutes an important task that needs to be addressed.

### 3. The Landau-Devonshire Multi-Well Potential

In order to complete the formulation of equations for the dynamics of SMA, we apply the method originally proposed by Landau and Khalatnikov (see Penrose and Fife [11] and references therein). In this method it is assumed that the state of the system at any given time can be described by an order parameter  $\varphi(\mathbf{x}, \theta)$  ( $\mathbf{x}$  is the position vector,  $\theta$  is the temperature), and that for all times (including times when the system is not in equilibrium) the free energy can be written in the form of a functional of  $\varphi(\mathbf{x}, \theta)$

$$\mathcal{E}_{L-K}[\varphi] = \int_{\Omega} \bar{F}(\varphi, \nabla_{\mathbf{x}}\varphi, \theta) d\mathbf{x}, \quad \bar{F} \equiv F(\varphi(\mathbf{x}, \theta)) + k(\theta)\tilde{F}(\nabla_{\mathbf{x}}\varphi(\mathbf{x}, \theta)). \quad (2)$$

In other words, the free energy density is assumed to be a potential in the form  $\bar{F}$ . In (2)  $\Omega$  is the fixed region of space occupied by the system,  $k$  is a positive coefficient,  $F$  is the local Helmholtz-type free energy density, and  $\tilde{F}$  is the Ginzburg-type term, often set to  $\tilde{F} = |\nabla_{\mathbf{x}}\varphi(\mathbf{x})|^2$  with  $k = \gamma/2$ , where  $\gamma$  is the Ginzburg coefficient (see details in Melnik et al [10]). As we noted in Melnik et al [10], with reported values of this coefficient ( $\gamma \propto 10^{-10} - 10^{-12}$ ) this term shows little influence on the dynamic of shape memory alloys. Therefore, in what follows we set  $\bar{F} = F$ , where, according to the Landau theory,  $F$  is a *non-convex* function.

A closely related approach to modelling crystalline solids that undergo phase transformations is based on considering elastic energy functionals such as the Ericksen-James energy functional,  $\mathcal{E}_{E-J}(\varphi) = \int_{\Omega} \tilde{F}(\nabla_{\mathbf{x}}\tilde{\varphi}(\mathbf{x})) d\Omega$ , where  $\tilde{F}(\cdot)$  is the non-convex energy density and  $\tilde{\varphi}$  is admissible deformations (see Li and Luskin [7], e.g.). Using this approach, a lot of attention (e.g. Bhattacharya et al [1]) was given to martensitic crystals that undergo an orthorhombic-to-monoclinic transformations (the case of "double-well" potential). However, for the appropriate description of solid-solid phase transitions even in the 1D case we are required to consider 3 equilibrium states (1 austenite and 2 twin martensites). This leads to the "triple-well" structure of the free energy function. This situation is typical for the microscopic level of modelling of SMA

phase transitions during which the cubic unit cell of austenite deforms tetragonally by Bain strain. However, at the mesoscopic level (of a few nm) the most typical change of symmetry during austenitic-martensitic phase transformations in SMA are cubic-to-monoclinic phase transformations (see Falk [5]). These transformations are the main focus of this paper where it is assumed that a cubic body centered crystal (b.c.c.) lattice with the crystallographic (habit) plane near  $\{110\}$  is transformed with a shear deformation on this plane (which coincides with the contact plane of austenite and martensite). Using the Falk approach developed in the 1D case, the free energy function is chosen in the Landau-Devonshire form that allows us to account quite well for the experimentally observed behaviour:

$$\Psi(\theta, \epsilon) = \psi_0(\theta) + \psi_1(\theta)\psi_2(\epsilon) + \psi_3(\epsilon), \quad (3)$$

where  $\psi_0(\theta) = \alpha_0 - \alpha_1\theta \ln \theta$  models thermal field contributions,  $\psi_1(\theta)\psi_2(\epsilon) = \alpha_2\theta\epsilon^2/2$  models shape-memory contributions, and  $\psi_3(\epsilon) = -\alpha_2\theta_1\epsilon^2/2 - \alpha_4\epsilon^4/4 + \alpha_6\epsilon^6/6$  models mechanical field contributions ( $\alpha_i$  and  $\theta_1$  are positive constants). Minima of this nonconvex free energy function are known to correspond different phases of the material (e.g. Liang and Rogers [8]). Depending on the value of temperature, the material may alternate between a single thermodynamically unstable nonmonotone branch and multiple unstable branches.

#### 4. Hyperbolic Approximations of SMA Dynamics

We chose the Cattaneo-Vernotte model for the heat conduction law and assume the strain-stress relation in the form

$$s = \rho \left[ p(\theta, \epsilon) + \lambda \left( \frac{\partial \theta}{\partial t}, \frac{\partial \epsilon}{\partial t} \right) \right], \quad p(\theta, \epsilon) = \frac{\partial \Psi}{\partial \epsilon}, \quad (4)$$

where  $\lambda$  is a function that depends on the rate of deformation gradient (with the constant of proportionality  $\mu$ ) and the rate of temperature (with the constant of proportionality  $\nu$ ). Then, the (nonlocal) model (1) can be reduced to the following one-dimensional hyperbolic approximation of SMA dynamics with respect to  $(u, \theta)$ :

$$\begin{cases} C_v \left[ \frac{\partial \theta}{\partial t} + \tau_0 \frac{\partial^2 \theta}{\partial t^2} \right] - k_1 \left[ \theta \frac{\partial u}{\partial x} \frac{\partial^2 u}{\partial t \partial x} + \tau_0 \frac{\partial}{\partial t} \left( \theta \frac{\partial u}{\partial x} \frac{\partial^2 u}{\partial t \partial x} \right) \right] - \mu \left[ \left( \frac{\partial^2 u}{\partial t \partial x} \right)^2 \right. \\ \left. + \tau_0 \frac{\partial}{\partial t} \left( \frac{\partial^2 u}{\partial t \partial x} \right)^2 \right] - \nu \left[ \frac{\partial \theta}{\partial t} \frac{\partial^2 u}{\partial t \partial x} + \tau_0 \frac{\partial}{\partial t} \left( \frac{\partial \theta}{\partial t} \frac{\partial^2 u}{\partial t \partial x} \right) \right] - \frac{\partial}{\partial x} \left( k \frac{\partial \theta}{\partial x} \right) = G, \\ \rho \frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x} \left[ k_1 \frac{\partial u}{\partial x} (\theta - \theta_1) - k_2 \left( \frac{\partial u}{\partial x} \right)^3 + k_3 \left( \frac{\partial u}{\partial x} \right)^5 \right] \\ - \mu \frac{\partial^3 u}{\partial x^2 \partial t} - \nu \frac{\partial^2 \theta}{\partial x \partial t} = F, \end{cases} \quad (5)$$

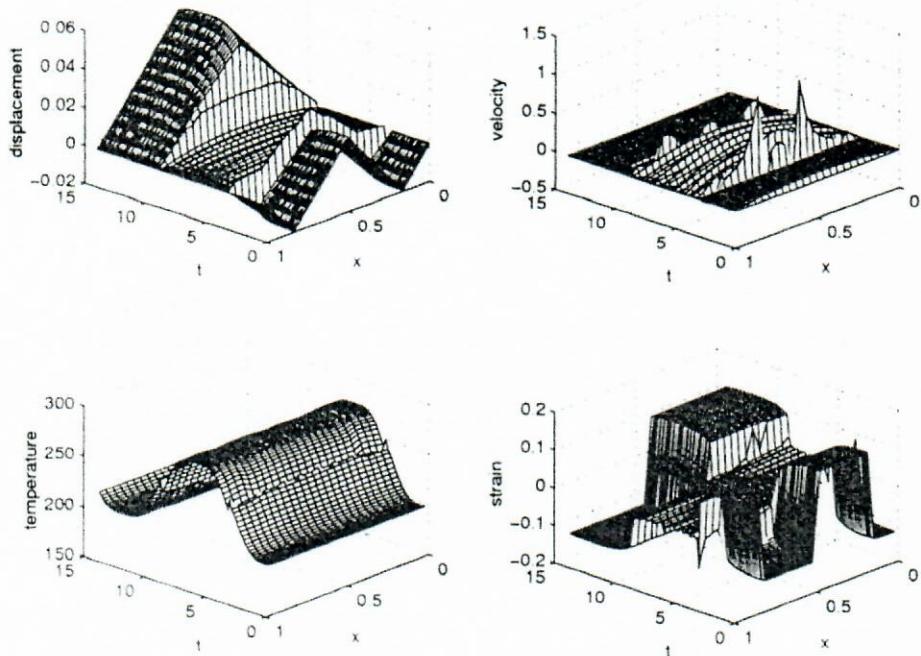


Figure 2: Thermally induced phase transformations.

where  $C_v$ ,  $\tau_0$ ,  $k$ ,  $k_1$ ,  $k_2$ ,  $k_3$ ,  $\mu$ ,  $\nu$  are given constants, and  $F$ ,  $G$  are given functions (see details in Melnik et al [10, 9]).

The system (5) is supplemented by appropriate initial and boundary conditions, and then, under some simplifying assumptions, is analysed by using the Leray-Schauder principle and the technique, based on the use of the Lumer-Phillips theorem (see Chen and Hoffmann [3]).

The numerical analysis of model (5) has been conducted via its reduction to a system of differential-algebraic equations with respect to  $u$ ,  $v$ ,  $\theta$ , and  $s$ . A typical result of computations for a  $\text{Au}_{23}\text{Cu}_{30}\text{Zn}_{47}$  rod of  $L = 1\text{cm}$  in length is presented in Fig. 2. The plot demonstrates a transformation from the martensite to austenite and then, upon cooling, back to a different martensite configuration (the stable attractor). Further details on this transformation and other experiments on thermomechanical control of phase transformations in SMA can be found in Melnik et al [10, 9].

The analysis of one-dimensional SMA models can be extended to dimensions higher than one. This extension is discussed in the next section where our approach is based on the Falk-Konopka generalisation of the Landau theory.

## 5. Centre Manifold Reduction of the 3D Falk-Konopka Models

There are two main approaches to the modelling of SMA in higher dimensional spaces. Firstly, we can formulate a 3D incremental constitutive model for which direct numerical implementations can be performed by using Newton-Raphson iteration method (see Lagoudas et al [6] and references therein). The models of this type are most effective for the analysis of thermomechanical responses of SMA specimens. Secondly, we can fit observations of the dynamics of SMA phase transformations into a 3D free energy function, and then substitute it into the general coupled system (1) that contains the equation of motion and the energy balance equation. The latter approach is adopted in this paper. Mathematical description of the appropriate mesoscale measure is initiated from the polynomial approximation (with respect to an order parameter  $\varphi$ ) of the free energy function

$$\Psi(\epsilon, \theta) = \psi^0(\theta) + \sum_{i=1}^{\infty} \psi^i(\epsilon, \theta), \quad (6)$$

where  $\psi^n$ ,  $n = 1, 2, \dots$  are strain invariants that define independent material parameters of the  $n$ -th order. For the copper-based alloys it is possible to reduce the number of required parameters in (5) to only 10 material constants (in the general case, temperature dependent, see details in Melnik et al [9],

Falk [5])

$$\Psi = \psi^0(\theta) + \sum_{j=1}^3 \psi_j^2 \mathcal{I}_j^2 + \sum_{j=1}^5 \psi_j^4 \mathcal{I}_j^4 + \sum_{j=1}^2 \psi_j^6 \mathcal{I}_j^6. \quad (7)$$

Having the free energy function, we define the shear stress by its quasi-conservative component,  $s^q = \rho \frac{\partial \Psi}{\partial \epsilon}$ . The definition of the internal energy function as  $e = \Psi - \theta \frac{\partial \Psi}{\partial \theta}$ , and an approximation of the 3D Cattaneo-Vernotte equation as in Melnik et al [9] completes the formulation of the 3D model for the dynamics of SMA.

Considering a shape memory alloy slab (large in the  $x = x_1$  direction compared to its thickness of  $2b$  in the  $y = x_2$  direction), we reduce this model to a simpler model written in terms of the amplitudes of cross-sectional averages of critical quantities (denoted below by  $U_1$  and  $\Theta'$ ). This reduction is derived by expressing the physical fields in terms of asymptotic sums in these amplitudes and their longitudinal gradients. Using center manifold theory (see in Melnik et al [9] and references therein), we find the asymptotic approximation that solves the system (1) describing the dynamics of SMA. By adapting the analysis of general center manifold technique to the nonlinear dynamics of SMA, we develop the slow, sub-center manifold model. Our technique allows to derive systematically (up to the arbitrary order of accuracy) an accurate low-dimensional model for the description of thermomechanical behaviour of thin slabs in shape memory alloy materials. Here we present the form of such a model in the case where the slab is thin enough so that in effect  $b = 0$ . The model is given in the form easily amenable to computational implementation by using a differential-algebraic solver (see Melnik et al [9] for details)

$$\left\{ \begin{array}{l} \rho \frac{\partial V_1}{\partial t} = \frac{\partial s}{\partial x} + F, \quad \frac{\partial U_1}{\partial t} = V_1, \\ C_v \frac{\partial \Theta'}{\partial t} = k \frac{\partial^2 \Theta'}{\partial x^2} + (c_{11} + c_{12}\Theta' - c_{13}(\Theta')^2) \frac{\partial U_1}{\partial x} \frac{\partial V_1}{\partial x} + \\ \quad + (c_{14} + c_{15}\Theta') \frac{\partial V_1}{\partial x} \left( \frac{\partial U_1}{\partial x} \right)^3 + c_{18} \frac{\partial V_1}{\partial x} \left( \frac{\partial U_1}{\partial x} \right)^5 + G, \\ s = (c_1 + c_2\Theta' - c_3(\Theta')^2) \frac{\partial U_1}{\partial x} - (c_4 - c_5\Theta') \left( \frac{\partial U_1}{\partial x} \right)^3 + c_6 \left( \frac{\partial U_1}{\partial x} \right)^5, \end{array} \right. \quad (8)$$

where all coefficients  $c_i$  are given.

We note that in the presence of a time-dependent forcing, the system may substantially deviate from the slow manifold and the use of geometric projection of initial conditions is required to determine the forcing appropriate for

the model. In this case the boundary conditions for the model also require a special treatment (see Melnik et al [9] and references therein).

Having found the amplitudes from system (8), the approximate expressions (up to arbitrary order) for the displacement and temperature fields of the slow manifold can be easily found using the technique developed in Melnik et al [9]. Compared to the models derived from constitutive-law-based phenomenological macroscale formulations (which can provide accurate results for space-averaged transformations only), our reduced 3D mesoscopic model better reflects the physics of phase transformations. The results obtained with this model shows the increased superimposed elastic vibrations in the temperature and strain fields as compared to the 1D case where such vibrations were seen clearly in the velocity field only (see Fig. 2, Melnik et al [10]). These vibrations in the temperature and strain fields are result of a much more complicated nonlinear behaviour of the system compared to the one dimensional case. A relevant tool for the study of this behaviour is provided by Young measures.

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