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ON CONTINUITY CONDITIONS AT THE PHASE INTERFACE OF TWO-PHASE ELASTIC SHELLS

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Abstract: The general non-linear theory of elastic shells undergoing stress-induced phase transition of martensitic type is developed. Our formulation is based on the statically and kinematically exact shell model. We also take into account the strain energy density of capillarity type as well as forces and couples applied along the curvilinear phase interface itself. The boundary value problem is formulated in the weak form through the variational principle of stationary total potential energy. In particular, we derive the refined static continuity conditions at the coherent interface and at the interface incoherent in rotations.

Keywords: non-linear shell, phase transition, continuity conditions

1. Introduction

Some non-classical materials may undergo diffusionless phase transitions (PTs) of martensitic type. Several mechanical models of such processes are summarized in books, for example by Podstrigach and Povstenko (1985), Grinfeld (1991) and Romano (1993). In particular, Povstenko (1991) proposed to treat the surface interfaces and three-phase curvilinear junctions in 3D continuum as 2D and 1D continua of the Cosserat (1909), respectively.

Thin films made of shape memory alloys can considerable alter their shapes under appropriate environmental changes. To model PTs in such thin bodies Eremeyev and Pietraszkiewicz (2004) and Pietraszkiewicz *et al.* (2007) used the statically and kinematically exact theory of shells presented in books by Libai and Simmonds (1998) and Chróścielewski *et al.* (2004). In such a shell model the 2D equilibrium conditions are derived by a direct through-thee-thickness integration of the equilibrium conditions of 3D continuum mechanics. Within the shell model the PT occurs at a movable surface curve separating shell regions with different material phases. One has only to complete the relations of the non-linear theory of regular shells with appropriate continuity conditions at the curvilinear phase interface. These conditions are necessary and sufficient for establishing the position of the interface in the thermodynamic equilibrium state of the shell.

In this report the curvilinear phase interface is endowed with the curvilinear strain energy density modeling the generalized capillary type phenomena, in analogy to the 2D phenomena in 3D bodies discussed for example by Finn (1986) or Rusanov (2005). We also take into account additional forces and couples applied along the interface curve itself. These loads may result from exact reduction to the 1D problem of the 3D phenomenon in a thin tube about the interface surface curve performed in analogy to the results by Konopińska and Pietraszkiewicz (2007) for branching and self-intersecting shells. They may directly model also curvilinear defects of any nature in thin-walled structures, such as dislocations for example, see Gurtin (2000).

2. Weak formulation of the equilibrium BVP

Deformation of the elastic shell is described by the displacement vector $\boldsymbol{u} \in E$ and the proper orthogonal (rotation) tensor $\boldsymbol{Q} \in SO(3)$ of the shell base surface M, see Chróścielewski *et al.* (2004). In shells undergoing PT of martensitic type we also need to know the position vector $\boldsymbol{x}_C \in E$ of the phase interface curve $C \subset M$ in the undeformed placement, where E is the 3D vector space, see Eremeyev and Pietraszkiewicz (2004).

The equilibrium boundary value problem (BVP) for the shell with PT can be formulated in the weak form: Given the external resultant surface forces and couples find a solution $(\boldsymbol{u}, \boldsymbol{Q}, \boldsymbol{x}_C)$ in the configurational space $S\{M; E \times SO(3) \times E\}$ satisfying the kinematic boundary conditions $\boldsymbol{u} = \boldsymbol{u}^*, \boldsymbol{Q} = \boldsymbol{Q}^*$ along $\partial M_d = \partial M \setminus \partial M_f$ such that for any kinematically admissible virtual displacement field $\{\delta \boldsymbol{u}, \boldsymbol{w} = ax(\delta \boldsymbol{Q}\boldsymbol{Q}^T), \delta \boldsymbol{x}_C\}$ the following principle of the total potential energy is satisfied:

$$\delta I = 0\,, \quad I = \iint_{M_A} W_A \mathrm{d}a + \iint_{M_B} W_B \mathrm{d}a + \int_C W_C \mathrm{d}s - A\,. \tag{2.1}$$

Here $W_A = W_A(\boldsymbol{E}, \boldsymbol{K})$ and $W_B = W_B(\boldsymbol{E}, \boldsymbol{K})$ are the 2D elastic strain energy densities associated with the subregions M_A and M_B of M with different material phases, respectively. The densities W_A and W_B depend only on the surface natural strain and bending tensors $\boldsymbol{E}, \boldsymbol{K} \in E \otimes T_x M$. $W_C = W_C(\boldsymbol{\varepsilon}, \boldsymbol{\kappa})$ is the 1D elastic strain energy density associated with the undeformed phase interface curve C itself. In general, W_C can be assumed to depend upon the natural curvilinear strain and bending tensors $\boldsymbol{\varepsilon}, \boldsymbol{\kappa} \in E \otimes T_x C$ of the interface C given for example in Chróścielewski et al. (2004).

In (2.1), A is the potential of external loads such that

$$\begin{aligned} \delta A = & \iint_{M \setminus C} (\boldsymbol{f} \bullet \delta \boldsymbol{u} + \boldsymbol{c} \bullet \boldsymbol{w}) \mathrm{d}a + \int_C (\boldsymbol{f}_C \bullet \delta \boldsymbol{u}_C + \boldsymbol{c}_C \bullet \boldsymbol{w}_C) \mathrm{d}a \\ & + \int_{\partial M_f} (\boldsymbol{n}^* \bullet \delta \boldsymbol{u} + \boldsymbol{m}^* \bullet \boldsymbol{w}) \mathrm{d}a + \boldsymbol{n}_e^* \bullet \delta \boldsymbol{u}_e + \boldsymbol{m}_e^* \bullet \boldsymbol{w}_e - \boldsymbol{n}_i^* \bullet \delta \boldsymbol{u}_i - \boldsymbol{m}_i^* \bullet \boldsymbol{w}_i\,. \end{aligned} \tag{2.2}$$

Here $\delta \boldsymbol{u}_C$ and $\boldsymbol{w}_C$ are the virtual translation and rotation vectors of the interface curve C, with $\delta \boldsymbol{u}_i, \boldsymbol{w}_i$ and $\delta \boldsymbol{u}_e, \boldsymbol{w}_e$ denoting the corresponding virtual displacements at the initial and end points of intersection of C with the boundary contour ∂M, respectively. The principle (2.1) with (2.2) states that among all possible values of $\boldsymbol{u}, \boldsymbol{Q}$ in $M \setminus C$ and positions $\boldsymbol{x}_C$ of the interface C the actual solution $\{\boldsymbol{u}^s, \boldsymbol{Q}^s, \boldsymbol{x}_C^s\}$ renders the functional stationary.

Calculating δI with I given by $(2.1)_2$ and (2.2) consists of two parts. In the first part we just refer to all transformations given in detail by Eremeyev and Pietraszkiewicz (2004) for I without the integral along C in $(2.1)_2$ as well as without the integral along C and the out-of-integral terms in (2.2). Variation of the integral along C in $(2.1)_2$, performed with the help of theorems for differentiation of curvilinear integrals over the time-dependent singular surface curve C given in Podstrigach and Povstenko (1985) and Cermelli *et al.* (1998), leads to

$$\begin{aligned}\delta \int_C W_C \mathrm{d}s &= \int_C (\boldsymbol{n} \bullet \delta^c \boldsymbol{\varepsilon} + \boldsymbol{m} \bullet \delta^c \boldsymbol{\kappa}) \,\mathrm{d}s + \int_C k_g V W_C \,\mathrm{d}s + W_C \delta \boldsymbol{x}_C \bullet \boldsymbol{\tau} \Big|_{x_i}^{x_e} \\ &= (\boldsymbol{n} \bullet \delta \boldsymbol{u}_C + \boldsymbol{m} \bullet \boldsymbol{w}_C) \Big|_{x_i}^{x_e} - \int_C \{\boldsymbol{n}' \bullet \delta \boldsymbol{u}_C + (\boldsymbol{m}' + \boldsymbol{y}_C' \times \boldsymbol{n}) \bullet \boldsymbol{w}_C\} \,\mathrm{d}s \\ &\quad + \int_C k_g V W_C \,\mathrm{d}s + W_C \delta \boldsymbol{x}_C \bullet \boldsymbol{\tau} \Big|_{x_i}^{x_e} .\end{aligned} \tag{2.3}$$

In (2.3), δ^c is the corotational variation, k_g is the geodesic curvature of C, $V = \delta \boldsymbol{x}_C \bullet \boldsymbol{\nu}$, $\boldsymbol{\nu} \in T_x M$ is the external unit normal to C, $\boldsymbol{\tau} = \boldsymbol{x}_C'$ is the unit tangent to C, $\delta^c \boldsymbol{\varepsilon}$ and $\delta^c \boldsymbol{\kappa}$ are given in Chróścielewski et al. (2004), and the stress resultant and stress couple vectors along C are defined by $\boldsymbol{n} = \partial W_C / \partial \boldsymbol{\varepsilon}$ and $\boldsymbol{m} = \partial W_C / \partial \boldsymbol{\kappa}$, respectively.

Introducing (2.3) and (2.2) into $(2.1)_1$ and using the results of Eremeyev and Pietraszkiewicz (2004) we obtain

$$\begin{aligned}\delta I = &-\iint_{M \setminus C} \Big((Div_s \boldsymbol{N} + \boldsymbol{f}) \bullet \delta \boldsymbol{u} + \{Div_s \boldsymbol{M} + ax(\boldsymbol{N}\boldsymbol{F}^T - \boldsymbol{F}\boldsymbol{N}^T) + \boldsymbol{c}\} \bullet \boldsymbol{w} \Big) \mathrm{d}a \\ &+ \int_{\partial M_f} \{(\boldsymbol{n}_\nu - \boldsymbol{n}^*) \bullet \delta \boldsymbol{u} + (\boldsymbol{m}_\nu - \boldsymbol{m}^*) \bullet \boldsymbol{w}\} \,\mathrm{d}s \\ &+ \int_{\partial M_d} (\boldsymbol{n}_\nu \bullet \delta \boldsymbol{u} + \boldsymbol{m}_\nu \bullet \boldsymbol{w}) \,\mathrm{d}s \\ &- \int_C \{V[W] - k_g V W_C + [\boldsymbol{n}_\nu \bullet \delta \boldsymbol{u}] + [\boldsymbol{m}_\nu \bullet \boldsymbol{w}] \\ &\qquad + (\boldsymbol{n}' + \boldsymbol{f}_C) \bullet \delta \boldsymbol{u}_C + (\boldsymbol{m}' + \boldsymbol{y}_C' \times \boldsymbol{n} + \boldsymbol{c}_C) \bullet \boldsymbol{w}_C\} \mathrm{d}s \\ &+ (\boldsymbol{n}_e - \boldsymbol{n}_e^*) \bullet \delta \boldsymbol{u}_e + (\boldsymbol{m}_e - \boldsymbol{m}_e^*) \bullet \boldsymbol{w}_e - (\boldsymbol{n}_i - \boldsymbol{n}_i^*) \bullet \delta \boldsymbol{u}_i - (\boldsymbol{m}_i - \boldsymbol{m}_i^*) \bullet \boldsymbol{w}_i \\ &+ W_{Ce} \delta \boldsymbol{x}_{Ce} \bullet \boldsymbol{\tau}_e - W_{Ci} \delta \boldsymbol{x}_{Ci} \bullet \boldsymbol{\tau}_i = 0 ,\end{aligned} \tag{2.4}$$

where $\boldsymbol{F} = Grad_s \boldsymbol{y}$ is the surface deformation gradient, $\boldsymbol{N} = \partial W / \partial \boldsymbol{E}$ and $\boldsymbol{M} = \partial W / \partial \boldsymbol{K}$ are the shell stress resultant and stress couple tensors of the Kirchhoff type for which the constitutive equations were discussed by Eremeyev and Pietraszkiewicz (2006), $\boldsymbol{n}_\nu = \boldsymbol{N}\boldsymbol{\nu}$ and $\boldsymbol{m}_\nu = \boldsymbol{M}\boldsymbol{\nu}$, the expression $[...] = (...)^+ - (...)^-$ means the jump at C, while $Grad_s$ and Div_s are the surface gradient and divergence operators on M, respectively.

Vanishing of the first two rows of (2.4) gives the known exact equilibrium equations and static boundary conditions of the general theory of regular shells, see Libai and Simmonds (1998) or Chróścielewski *et al.* (2004). The third and sixth rows of (2.4) vanish identically along ∂M_d where the kinematic boundary conditions are satisfied. The last terms in (2.4) vanish identically if the end points x_e and x_i of C belong to ∂M_d. When $(x_{Ci}, x_{Ce}) \in \partial M_f$ these terms also vanish if $\delta \boldsymbol{x}_{Ci}$ and $\delta \boldsymbol{x}_{Ce}$ are normal to C. We are not aware of any physical process of PT in shells which would require taking into account that $\delta \boldsymbol{x}_C \bullet \boldsymbol{\tau} \neq 0$ at the end points of C. Therefore, we assume that $\delta \boldsymbol{x}_{Ci} \bullet \boldsymbol{\tau}_i = \delta \boldsymbol{x}_{Ce} \bullet \boldsymbol{\tau}_e \equiv 0$ and omit terms of the last row of (2.4) from further considerations. As a result, these terms do not influence the thermodynamic equilibrium conditions of the two-phase shell.

3. Static continuity conditions

In this paper we discuss only such types of PT which do not lead to fragmentation of the shell. This is possible in two types of PT.

The phase interface is called *coherent* if both fields $\boldsymbol{y}$ and $\boldsymbol{Q}$ are continuous at C:

$$\begin{aligned} &\boldsymbol{y}^- = \boldsymbol{y}^+ = \boldsymbol{y}_C, \quad [\boldsymbol{y}] = \boldsymbol{0}, \quad [\boldsymbol{y}'] = \boldsymbol{0}, \\ &\boldsymbol{Q}^- = \boldsymbol{Q}^+ = \boldsymbol{Q}_C, \quad [\boldsymbol{Q}] = \boldsymbol{0}, \quad [\boldsymbol{Q}'] = \boldsymbol{0}. \end{aligned} \tag{3.1}$$

The coherent phase interface may be singular with regard to $\boldsymbol{F}$ and $Grad_s \boldsymbol{Q}$, but not with regard to $\boldsymbol{y}$ and $\boldsymbol{Q}$ themselves. Then from the Maxwell theorem we establish the local kinematic compatibility conditions along C, see Eremeyev and Pietraszkiewicz (2004),

$$[\delta \boldsymbol{u}] + V[\boldsymbol{F}\boldsymbol{\nu}] = \boldsymbol{0}, \quad [\boldsymbol{w}] + V[\boldsymbol{K}\boldsymbol{\nu}] = \boldsymbol{0}, \tag{3.2}$$

which relate $[\delta \boldsymbol{u}]$ and $[\boldsymbol{w}]$ with V. Therefore, along the coherent interface only the virtual fields $V, \delta \boldsymbol{u}_C, \boldsymbol{w}_C$ are independent. For such an interface from the fourth, fifth and sixth rows of (2.4) after some transformations we obtain the local static continuity conditions along C

$$\begin{aligned} &[W] - \langle \boldsymbol{N}\boldsymbol{\nu} \rangle \bullet [\boldsymbol{F}\boldsymbol{\nu}] - \langle \boldsymbol{M}\boldsymbol{\nu} \rangle \bullet [\boldsymbol{K}\boldsymbol{\nu}] = k_g W_C, \\ &\boldsymbol{n}' + [\boldsymbol{N}\boldsymbol{\nu}] + \boldsymbol{f}_C = \boldsymbol{0}, \quad \boldsymbol{m}' + \boldsymbol{y}_C' \times \boldsymbol{n} + [\boldsymbol{M}\boldsymbol{\nu}] + \boldsymbol{c}_C = \boldsymbol{0}. \\ &\boldsymbol{n}_i - \boldsymbol{n}_i^* = \boldsymbol{0}, \quad \boldsymbol{m}_i - \boldsymbol{m}_i^* = \boldsymbol{0} \quad \text{at } x_i = C \cap \partial M_f, \\ &\boldsymbol{n}_e - \boldsymbol{n}_e^* = \boldsymbol{0}, \quad \boldsymbol{m}_e - \boldsymbol{m}_e^* = \boldsymbol{0} \quad \text{at } x_e = C \cap \partial M_f, \end{aligned} \tag{3.3}$$

where $\langle ... \rangle = \frac{1}{2}\{(...)^{+} + (...)^{-}\}$ is the mean value at C.

The phase interface is called *incoherent in rotations* if only $\boldsymbol{y}$ is continuous at C but the continuity of $\boldsymbol{Q}$ may be violated. In this case the conditions indicated in the first row of (3.1) are still satisfied, but those in the second row of (3.1) may be violated. Such an interface can be singular with regard to $\boldsymbol{Q}, \boldsymbol{F}$, and $Grad_s \boldsymbol{Q}$ but not with regard to $\boldsymbol{y}$ and the second kinematic compatibility condition (3.2) can now be violated. As a result, along the interface incoherent in rotations the virtual fields $V, \boldsymbol{w}^{\pm}, \delta \boldsymbol{u}_C$, and $\boldsymbol{w}_C$ are independent. At such an interface after appropriate transformations we obtain the following set of local static continuity conditions

$$\begin{aligned} &[W] - \langle \boldsymbol{N}\boldsymbol{\nu} \rangle \bullet [\boldsymbol{F}\boldsymbol{\nu}] = k_g W_C , \quad \boldsymbol{M}^{\pm}\boldsymbol{\nu} = \boldsymbol{0} , \\ &\boldsymbol{n}' + [\boldsymbol{N}\boldsymbol{\nu}] + \boldsymbol{f}_C = \boldsymbol{0} , \quad \boldsymbol{m}' + \boldsymbol{y}'_C \times \boldsymbol{n} + \boldsymbol{c}_C = \boldsymbol{0} , \end{aligned} \tag{3.4}$$

together with static continuity conditions at the initial and end points of C given in the third and fourth row of (3.3).

4. Capillary energy of the interface

Let us consider a special case of curvilinear strain energy density W_C of the phase interface by analogy to the one used in the theory of capillary surfaces, see Finn (1986) and Rusanov (2005). In our 1D case the term responsible for the curvilinear energy in the functional (2.1) can be assumed to be given by the integral $\sigma \int_C \sqrt{\boldsymbol{y}'_C \cdot \boldsymbol{y}'_C}\, ds$ so that

$$W_C = \sigma \sqrt{\boldsymbol{y}'_C \cdot \boldsymbol{y}'_C} . \tag{4.1}$$

Here σ is the line tension which is constant along the deformed curvilinear interface $D = \chi(C)$. Other possible types of constitutive equations of one-dimensional continua modeling the curvilinear interface can be found in Podstrigach and Povstenko (1985). The concept of line tension is widely used not only in the theory of capillarity but also in the theory of dislocations, where the line tension takes into account the energy of a tube surrounding the dislocation.

When the strain energy density (4.1) is used we can simplify the continuity conditions along the phase interface (3.3) and (3.4). Indeed, from the equation (4.1) we obtain

$$\boldsymbol{n} = \frac{\sigma}{\sqrt{\boldsymbol{y}'_C \bullet \boldsymbol{y}'_C}} \boldsymbol{y}'_C , \quad \boldsymbol{m} = \boldsymbol{0} . \tag{4.2}$$

Thus, using (4.2) we find that $\boldsymbol{n}\times\boldsymbol{y}'_C=\boldsymbol{0}$. If we further assume that $\boldsymbol{c}_C=\boldsymbol{0}$ the third equation of (3.3) reduces to $[\boldsymbol{M}\boldsymbol{\nu}]=\boldsymbol{0}$ while the fourth one of (3.4) becomes identically satisfied.

Note that $\boldsymbol{y}'_C/\sqrt{\boldsymbol{y}'_C\cdot\boldsymbol{y}'_C}$ is the unit vector tangent to the interface curve D. Then from the Frénet formulas it follows that

$$\left(\frac{1}{\sqrt{\boldsymbol{y}'_C\cdot\boldsymbol{y}'_C}}\boldsymbol{y}'_C\right)'=k\sqrt{\boldsymbol{y}'_C\cdot\boldsymbol{y}'_C}\,\boldsymbol{\mu}\,, \tag{4.3}$$

where k is the principal curvature of the interface curve D, and $\boldsymbol{\mu}$ is the principal unit normal to D. Then with the additional assumption that $\boldsymbol{f}_C=\boldsymbol{0}$ the second equation of (3.3) or the third one of (3.4) reduces to

$$\sigma k\sqrt{\boldsymbol{y}'_C\cdot\boldsymbol{y}'_C}\,\boldsymbol{\mu}+[\boldsymbol{N}\boldsymbol{\nu}]=\boldsymbol{0}\,. \tag{4.4}$$

The equation (4.4) is a 1D analog of the Laplace equation well-known in the 2D theory of capillarity, see Finn (1986) and Rusanov (2005).

5. Conclusions

The equilibrium boundary value problem of elastic shells undergoing phase transitions of martensitic type has been developed. In our approach the statically and kinematically exact theory of shells of the Cosserat type has been used. The phase transition has been assumed to take place at the movable singular surface curve. From the variational principle of stationary total potential energy we have derived not only the local equilibrium conditions of the regular shell parts, but also the local continuity conditions at the coherent phase interface and at the interface incoherent in rotations. These continuity conditions allow one to establish position of the interface curve in the thermodynamic equilibrium state. Numerical examples of the phase transition in an infinite plate with a circular hole given in Eremeyev and Pietraszkiewicz (2004) and Pietraszkiewicz *et al.* (2007) illustrate the results presented in this report.

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