Phase Transitions in Thermoviscoelastic Shells

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Definition

A phase transition is the transformation of a thermodynamic system from one state of matter to another. In shell structures it consists primarily of a diffusionless displacive change of the material lattice. Such phase transition process can usually be induced by changing the temperature or by applying an external stress. Experiments indicate that the new solid phase nucleates in narrow regions across which large changes occur in some material properties. Thus, the two-phase shell can be regarded as a deformable material surface consisting of two material phases divided by a movable non-material surface curve.

Overview

The interest in thin-walled structures undergoing phase transitions (PT) grows recently from their prospective applications in engineering. As examples of such structures martensitic films and biological membranes can be considered. The stress- and temperature-induced PT are widely observed in thin-walled structures made of superelastic shape memory alloys (SMA) and shape memory polymers, such as NiTi, NiMnGa, AgCd, AuCd, CuAlNi, polyurethane, etc, which are used in various microelectromechanical systems (MEMS). Thin plates, strips, and tubes made of SMA are used as working elements of such MEMS as micropumps, sensors, actuators, microengines etc., see [1, 2].

The major known theories of PT in deformable solids are related to threedimensional (3D) thermoelasticity, see [1,3,4] and references given therein. Simple two-dimensional (2D) mechanical models of PT in thin films are presented in $[1, 2]$.

The non-linear resultant equilibrium conditions of elastic shells undergoing PT of martensitic type were formulated in [5] within the resultant dynamically exact and kinematically unique theory of shells presented in [6, 7]. These conditions were extended in [8] by taking into account the line tension energy of the interface and in [9, 10] to thermoviscoelastic shells. By analogy to the 3D case, the two-phase shell was regarded in [5, 8–10] as a deformable surface consisting of two material phases divided by a sufficiently smooth surface singular curve (phase interface). Several experiments on thin-walled plates, strips, and tubes demonstrate how the macroscopic domain of the new phase forms, show its further evolution during loading and annihilation after unloading. In the case of plates and strips the new phase forms often as a few bands across the strip. In the case of tubes the new phase may also appear as helical or cylindrical bands which width and shape depend on geometric and material parameters, acting loads and temperature. Other examples of PT in thin-walled structures are tents and tunnels appearing in martensitic thin films, see [11].

Here we present the resultant 2D thermomechanics of shells undergoing diffusionless, displacive phase transitions of martensitic type of the shell material and formulate the corresponding non-linear boundary-value problem (BVP).

Kinematics of resultant theory of shells

Kinematics of the general resultant 2D theory of shells coincides with the kinematics of 2D Cosserat continuum, see [6, 7] for details. In the undeformed placement the shell is represented by the base surface M with the position vector $x(\theta^\alpha)$ and the unit normal vector $n(\theta^{\alpha})$, where $\{\theta^{\alpha}\}, \alpha = 1, 2$, are surface curvilinear coordinates, see Fig. 1. In the deformed placement the shell is represented by the surface $N = \chi(M)$ with the position vector $y = \chi(x)$ and the attached three directors (d_{α}, d) . Deformation of the shell is described by the relations

$$
\mathbf{y}(\mathbf{x},t) = \mathbf{\chi}(\mathbf{x}) = \mathbf{x} + \mathbf{u}(\mathbf{x},t), \quad \mathbf{d}_{\alpha}(\mathbf{x},t) = \mathbf{Q}(\mathbf{x},t)\mathbf{x}_{,\alpha}, \quad \mathbf{d}(\mathbf{x},t) = \mathbf{Q}(\mathbf{x},t)\mathbf{n}(\mathbf{x}), \tag{1}
$$

where *t* is a time-like scalar parameter, χ the deformation function, \boldsymbol{u} the translation vector of *M*, and $Q \in SO(3)$ the proper orthogonal tensor representing the work-averaged gross rotation of the shell cross sections from their undeformed shapes described by (x, α, n) , where $(.)_{,\alpha}$ denotes partial differentiation with respect to θ^{α} . Then $\mathbf{v} \equiv \dot{\mathbf{u}}$ is the translation velocity and $\mathbf{\omega} \equiv \text{ax}(\dot{Q}Q^{T})$ the angular velocity vectors, where $ax(...)$ is the axial vector associated with the skew tensor $(...)$, and $\dot{(.)}$ denotes the derivative with respect to *t*.

Within the framework of resultant theory of shells considered here, the two strain measures corresponding to the deformations (1) are, see [5, 7]:

$$
E = \boldsymbol{\varepsilon}_{\alpha} \otimes \boldsymbol{a}^{\alpha}, \quad K = \boldsymbol{\varkappa}_{\alpha} \otimes \boldsymbol{a}^{\alpha}, \quad \boldsymbol{\varepsilon}_{\alpha} = \boldsymbol{y}_{,\alpha} - \boldsymbol{d}_{\alpha}, \quad \boldsymbol{\varkappa}_{\alpha} = \frac{1}{2} \boldsymbol{d}^{i} \times \boldsymbol{Q}_{,\alpha} \boldsymbol{Q}^{T} \boldsymbol{d}_{i}, \quad (2)
$$

Figure 1: Kinematics of a two-phase shell

where (a^{α}, n) and (d^{i}) , $i = 1, 2, 3$, are bases reciprocal to the bases (x, α, n) and (d_{α}, d) , respectively, and \otimes is the tensor product. In (2) and below quantities with repeated upper and lower Greek or Latin indices are summed over range of the indices.

We assume that in the deformed placement the shell base surface *N* consists of different material phases occupying different complementary subregions separated by the curvilinear phase interface $D \in N$, see Fig. 1. For a piecewise differentiable mapping χ we can introduce on *M* a singular image curve $C = \chi^{-1}(D)$ with the position vector x_C . We call a priori unknown curves *D* and *C* the phase interfaces in the deformed and reference placements, respectively. Let us note that x_C and y_D are kinematically independent on *u* and *Q*. This means that *D* and *C* are non-material surface curves, in general. For the description of quasistatic motion of *C* on *M* we introduce the phase interface velocity $V \equiv \dot{x}_C \cdot \mathbf{v}$, where $\mathbf{v} \in T_xM$ is the unit external normal vector to *C*, and $\mathbf{v} \cdot \mathbf{n} = 0$, while T_xM is the tangent space to *M* at *x*. Hence, *y* (or *u*), *Q*, and x_C constitute the basic kinematic unknowns of the non-linear resultant theory of shells undergoing PT.

Integral balance laws and entropy inequality

The resultant 2D equations of the non-linear theory of shells can be derived by direct through-the-thickness integration of 3D balance laws of linear and angular momentum as well as of 3D energy balance and entropy inequality of continuum thermodynamics, see [5–7, 10, 12]. In quasi-static problems discussed here the global equilibrium conditions require the total force and total torque of all loads acting upon any part $P \subset M \backslash C$ to vanish,

$$
\mathbf{F} = \mathbf{0}, \quad \mathbf{M} = \mathbf{0}, \tag{3}
$$

^p

where

$$
\mathbf{F} \equiv \iint\limits_P f \, da + \int\limits_{\partial P \setminus \partial M_f} \mathbf{n}_v \, ds + \int\limits_{\partial P \cap \partial M_f} \mathbf{n}^* \, ds,
$$

$$
\mathbf{M} \equiv \iint\limits_P (c + \mathbf{y} \times \mathbf{f}) \, da + \int\limits_{\partial P \setminus \partial M_f} (\mathbf{m}_v + \mathbf{y} \times \mathbf{n}_v) \, ds + \int\limits_{\partial P \cap \partial M_f} (\mathbf{m}^* + \mathbf{y} \times \mathbf{n}^*) \, ds.
$$

Here f and c are the resultant surface force and couple vector fields acting on $N\backslash D$, but measured per unit area of $M\backslash C$. Similarly, n_v and m_v are the internal contact stress and couple resultant vectors defined at an arbitrary edge ∂R of $R = \chi(P)$, while n^* and m^* are the external boundary resultant force and couple vectors applied along the part ∂N_f of $N = \chi(M)$, respectively. The latter four vectors are measured per unit length of the corresponding undeformed edges [∂]*P* and [∂]*M^f* , respectively.

According to the Cauchy postulate, the contact vectors n_v and m_v can be represented through the respective internal surface stress and couple resultant tensors *N* and *M* by $n_v = Nv$, $m_v = Mv$. The tensors *N*, $M \in E \otimes T_xM$ defined on $M \setminus C$ are the resultant surface stress measures of the Piola type, respectively, and *E* is the 3D vector space.

In the literature several formulations of shell thermodynamics are known, where various surface fields responsible for temperature are used and several forms of the first and second laws of thermodynamics for shells are discussed.

The resultant local energy balance and entropy inequality for the shell can also be derived by direct through-the-thickness integration of the global 3D balance of energy and entropy inequality, see [10, 12, 13].

The referential form of energy balance *(The 1st Law of thermodynamics)* of an arbitrary part *P* of the shell base surface $M\$ C can be described in analogy to the 3D energy balance, see [14], by the resultant quantities as

$$
\dot{\mathbf{K}} + \dot{\mathbf{E}} = \mathbf{A} + \mathbf{Q},\tag{4}
$$

where K is the resultant kinetic energy, E is the resultant internal energy, A is the resultant mechanical power, and Q is the resultant heating. For the quasistatic process discussed here $\dot{K} \equiv 0$, while E, A, and O can be represented on any *P* ⊂ $M\backslash C$ by

$$
E \equiv \iint\limits_P \rho \varepsilon da, \quad A \equiv \iint\limits_P (f \cdot \mathbf{v} + c \cdot \boldsymbol{\omega}) da + \int\limits_{\partial P \setminus \partial M_f} (\mathbf{n}_v \cdot \mathbf{v} + \mathbf{m}_v \cdot \boldsymbol{\omega}) ds
$$

$$
+ \int\limits_{\partial P \cap \partial M_f} (\mathbf{n}^* \cdot \mathbf{v} + \mathbf{m}^* \cdot \boldsymbol{\omega}) ds,
$$

$$
Q \equiv \iint\limits_P \rho r da + \int\limits_{\partial P \setminus \partial M_h} q_v ds + \int\limits_{\partial P \cap \partial M_h} q^* ds,
$$

where ρ is the resultant surface mass density in undeformed placement, ε the resultant internal surface strain energy density per unit undeformed surface mass, and *r* the internal resultant surface heat supply minus heat fluxes through the upper and lower shell faces, all per unit mass of M , q_v and q^* are the surface heat fluxes through ∂P and ∂M_h , respectively. The contact heat flux q_v can be represented through the surface heat flux vector *q* by the formula $q_v = q \cdot v$.

The referential form of entropy inequality *(The 2nd Law of thermodynamics)* of an arbitrary part *P* of the shell base surface $M\setminus C$ follows from the Clausius-Duhem inequality [14],

$$
\dot{H} \geq J,\tag{5}
$$

where in our case H is the resultant shell entropy and J the resultant entropy supply. For any part $P \subset M \backslash C$ these fields are defined as follows:

$$
H \equiv \iint\limits_P \rho \eta \, da, \quad J \equiv \iint\limits_P \rho \, j \, da + \int\limits_{\partial P \setminus \partial M_h} j_V \, ds + \int\limits_{\partial P \cap \partial M_h} j^* \, ds,
$$

where η is the resultant internal entropy density, *j* the resultant entropy supply minus entropy fluxes through the upper and lower shell faces, both per unit undeformed surface mass, and j_v and j^* are the resultant entropy fluxes through the internal ∂P and external ∂M_h boundary contours, respectively. The field j_v

can be expressed through the referential entropy flux vector $j \in T_xM$ according to $j_v = j \cdot v$.

The relations between the resultant quantities and their 3D counterparts can be derived by use of the through-the-thickness integration procedure applied to the 3D fields, [10, 12].

On *M* we introduce the mean referential temperature $\theta(x,t) > 0$ and the temperature deviation $\varphi(x,t)$ by

$$
\frac{1}{\theta} = \frac{1}{2} \left(\frac{1}{\theta_+} + \frac{1}{\theta_-} \right), \quad \varphi = \frac{1}{h} \left(\frac{1}{\theta_-} - \frac{1}{\theta_+} \right), \tag{6}
$$

where $\theta_+ > 0$ are temperatures of the upper and lower shell faces M^{\pm} taken to be equal to those prevailing in the adjoining external media, and *h* is the shell thickness.

Unlike in the 3D entropy inequality [14], the resultant surface entropy supply *j* and flux vector *j* take now the extended forms

$$
j = \frac{1}{\theta}r - \varphi s, \quad j = \frac{1}{\theta}q - \varphi s,
$$
 (7)

where *s* is the resultant extra heat supply and *s* is the resultant extra heat flux vector.

Local shell equations and constitutive relations

From the integral 2D equilibrium equations (3), the energy balance equation (4) and the entropy inequality (5), after appropriate transformations follow the local Lagrangian equilibrium conditions

Div
$$
N+f=0
$$
, Div M + ax $(NFT - FNT)$ + c = 0 in $M\setminus C$,
\n $Nv - n^* = 0$, $Mv - m^* = 0$ along ∂M_f , (8)

the local thermomechanic balances of energy

$$
\rho \dot{\varepsilon} = \rho r - \text{Div}\, q + N \bullet E^{\circ} + M \bullet K^{\circ} \quad \text{in } M \setminus C, \nq \cdot \mathbf{v} - q^* = 0 \quad \text{along } \partial M_h,
$$
\n(9)

and the local resultant entropy inequalities

$$
\rho \dot{\eta} - \rho \left(\frac{r}{\theta} - \varphi s \right) + \frac{1}{\theta} \text{Div } q - \varphi \text{Div } s + \boldsymbol{h} \cdot s - \frac{1}{\theta^2} q \cdot g \ge 0 \quad \text{in} \quad M \setminus C,
$$
\n
$$
\frac{q^*}{\theta^*} - \varphi^* s^* - \left(\frac{q_V}{\theta} - \varphi s_V \right) \ge 0 \quad \text{along} \quad \partial M_h,
$$
\n
$$
g = \text{Grad } \theta, \quad \boldsymbol{h} = \text{Grad } \varphi, \qquad g, \boldsymbol{h} \in T_x M,
$$
\n(10)

of the non-linear resultant shell thermomechanics. Here $F \equiv$ Grad $y = y_{,\alpha} \otimes a^{\alpha}$ is the surface deformation gradient, $\bm{F}\in E\otimes T_xM$, $\textrm{Div}\bm{N}\!\equiv\!\bm{N}_{,\alpha}\!\cdot\!\bm{a}^{\alpha}$ means the surface divergence of *N*, $(\cdot)^{\circ} \equiv Q \frac{d}{dt} [Q^T(\cdot)]$ is the co-rotational time derivative, and the scalar product of two tensors $A, B \in E \otimes T_xM$ is defined by $A \bullet B \equiv \text{tr}(A^T \ B)$.

The fields u, Q, θ, φ constitute the basic thermo-kinematic independent variables of the shell boundary value problem in $M\setminus C$, while the fields $N, M, \varepsilon, \eta, \chi, q$, and *s* have to be specified by the constitutive equations.

The constitutive equations for thermoelastic shells take the form [10],

$$
\psi \equiv \varepsilon - \theta \eta - \varphi \chi = \psi(E, K, \theta, \varphi),
$$

\n
$$
N = \rho \psi_E, \quad M = \rho \psi_K, \quad \eta = -\psi_{,\theta}, \quad \chi = -\psi_{,\varphi},
$$

\n
$$
q = q(E, K, \theta, g, \varphi, h), \quad s = s(E, K, \theta, g, \varphi, h),
$$
\n(11)

where explicit expressions of the free energy ψ as well as for q and s follow from requirements of material frame-indifference and of the imposed material symmetry.

For thermoelastic shells the local energy balance equation (9) reduces to

$$
\rho(\theta \dot{\eta} + \varphi \dot{\chi}) = \rho r - \text{Div}\,\mathbf{q},\tag{12}
$$

while the local entropy inequality (10) results in the equation

$$
-\rho \dot{\chi} + \rho \theta s - \theta \text{Div} s = c\phi, \quad c \ge 0,
$$
 (13)

where the new constitutive function c is introduced, and the reduced dissipation inequality becomes

$$
-\frac{1}{\theta}\mathbf{g}\cdot\mathbf{q} - \theta\mathbf{h}\cdot\mathbf{s} \ge 0. \tag{14}
$$

Both relations (12) and (13) play the role of thermoconductivity equations in the theory of thermoelastic shells. The two equations are necessary to determine two fields: the surface mean temperature θ and the surface temperature deviation ϕ.

The thermoelastic constitutive equations (11) can be extended to the thermoviscoelastic ones which are important for example for description of shells made of shape memory polymers. A simple example of thermoviscoelastic shells is based on the Kelvin-Voigt type model. In this case the 2D stress measures *N* and *M* can be decomposed into the equilibrium and dissipative parts,

$$
N = N_E + N_D, \quad M = M_E + M_D,
$$

\n
$$
N_E = N_E(E, K, \theta, g, \varphi, h), \quad M_E = M_E(E, K, \theta, g, \varphi, h),
$$

\n
$$
N_D = N_D(E, K, E^{\circ}, K^{\circ}, \theta, g, \dot{\theta}, \dot{g}, \varphi, h, \dot{\varphi}, \dot{h}),
$$

\n
$$
M_D = M_D(E, K, E^{\circ}, K^{\circ}, \theta, g, \dot{\theta}, \dot{g}, \varphi, h, \dot{\varphi}, \dot{h}),
$$
\n(15)

where

$$
N_D(E, K, 0, 0, \theta, g, 0, 0, \phi, h, 0, 0) = 0, \quad M_D(E, K, 0, 0, \theta, g, 0, 0, \phi, h, 0, 0) = 0.
$$

In the case of Kelvin-Voigt type model the 2D free energy density ψ and the equilibrium surface stress measures N_E , M_E are the same as in the case of thermoelastic shells, while N_D , M_D , q , and s may depend on the full list of arguments including the temperature deviation φ , its surface gradient and their timelike derivatives. The reduced 2D dissipation inequality takes the form

$$
N_D \bullet E^{\circ} + M_D \bullet K^{\circ} - \frac{1}{\theta} g \cdot q - \theta h \cdot s \ge 0, \qquad (16)
$$

which puts a restriction placed on allowable forms of the response functions for N_D and M_D .

The simplest cases of the constitutive equations for *q* and *s* satisfying (14) or (16) may be taken similar to the referential Fourier law in 3D continuum thermodynamics,

$$
\boldsymbol{q} = -c_{\parallel} \boldsymbol{g}, \quad \boldsymbol{s} = -c_{\perp} \boldsymbol{h}, \tag{17}
$$

where c_{\parallel} is the positive heat conductivity of the shell in tangential direction and *c*[⊥] is the positive heat conductivity of the shell in the transverse normal direction.

Continuity conditions and kinetic equation

When a phase transition process takes place in the shell, some fields defined on *M* can be discontinuous across *C*. In particular, the curvilinear phase interfaces in shells can be either coherent or incoherent in rotations, see [5]. For the coherent interface both fields y (or u) and Q are supposed to be continuous at C and the kinematic compatibility conditions along *C* become

$$
[\![\mathbf{v}]\!] + V[\![F\mathbf{v}]\!] = \mathbf{0},\tag{18}
$$

$$
[\![\boldsymbol{\omega}]\!] + V[\![K\boldsymbol{v}]\!] = \mathbf{0},\tag{19}
$$

where the expression $[\![...]\!] = (\ldots)_{B} - (\ldots)_{A}$ means the jump at *C*.

The phase interface is incoherent in rotations if only *y* (or *u*) is continuous at *C* but *Q* may be discontinuous. In this case the condition (18) is still satisfied, but (19) may be violated, see [5].

Assuming $\llbracket y \rrbracket = \mathbf{0}$ along *C*, from (3) we obtain the local Lagrangian dynamic compatibility conditions [7],

$$
[[Nv]] = 0, \quad [[Mv]] = 0,
$$
\n(20)

which are just the local balances of forces and couples at *C* in the case of quasistatic deformations.

In PT problems of shells the mean referential temperature θ and its deviation ϕ are continuous on the whole *M*,

$$
[\![\theta]\!]=0, \quad [\![\varphi]\!]=0 \quad \text{along } C. \tag{21}
$$

The local jumps of energy balance and of entropy inequality along *C* corresponding to (4) and (5) are $[10]$,

$$
V[\![\rho \varepsilon]\!] + [\![N\mathbf{v} \cdot \mathbf{v}]\!] + [\![M\mathbf{v} \cdot \mathbf{\omega}]\!] - [\![q \cdot \mathbf{v}]\!] = 0,\tag{22}
$$

$$
V[\![\rho\eta]\!] - \left[\!\left[\frac{1}{\theta}\boldsymbol{q}\cdot\boldsymbol{v}\right]\!\right] + [\![\varphi s\cdot\boldsymbol{v}]\!] \equiv \delta_C^2 \geq 0, \qquad (23)
$$

where $\delta_C^2 \ge 0$ denotes the surface entropy production along *C*.

To the second thermoconductivity equation (13) there corresponds the jump relation along *C*,

$$
V\frac{1}{\theta}[\![\rho \chi]\!] - [\![s \cdot \mathbf{v}]\!] = 0. \tag{24}
$$

From (18) – (24) we obtain the compatibility condition in the form

$$
\theta \delta_C^2 = -V \left\{ \left[\left[\rho \psi \right] \right] - \mathbf{v} \cdot \mathbf{N}^T \left[\left[\mathbf{F} \mathbf{v} \right] \right] - \mathbf{v} \cdot \mathbf{M}^T \left[\left[\mathbf{K} \mathbf{v} \right] \right] \right\} \quad \text{along } C \tag{25}
$$

for the coherent phase interface, and

$$
\theta \delta_C^2 = -V \{ [\![\rho \psi]\!] - \mathbf{v} \cdot N^T [\![F \mathbf{v}]\!] \} \quad \text{along } C \tag{26}
$$

for the phase interface incoherent in rotations.

The entropy production δ_C^2 remains always non-negative for all thermomechanical processes. This allows us to postulate the kinetic equation, describing motion of the phase interface for all quasistatic processes, in the form

$$
V = -F\left(\mathbf{v} \cdot \left[\llbracket \mathbf{C} \rrbracket \mathbf{v}\right],\right) \tag{27}
$$

where F is the non-negative definite kinetic function depending on the jump of *C* at *C*, i.e. $F(\zeta) \ge 0$ for $\zeta > 0$, where $C = C_c \equiv \rho \psi A - N^T F - M^T K$ for the

coherent interface and $C = C_i \equiv \rho \psi A - N^T F$ for the one incoherent in rotations, $A = I - n \otimes n$, and **I** is the 3D identity tensor.

Following [3,4] we can take the kinetic function $F(\zeta)$ in the form

$$
F(\zeta) = \begin{cases} \frac{k(\zeta - \zeta_0)}{1 + \xi(\zeta - \zeta_0)} & \zeta \ge \zeta_0, \\ 0 & -\zeta_0 < \zeta < \zeta_0, \\ \frac{k(\zeta + \zeta_0)}{1 - \xi(\zeta + \zeta_0)} & \zeta \le -\zeta_0. \end{cases} \tag{28}
$$

Here ζ_0 describes the effects associated with nucleation of the new phase and action of the surface tension, see [3], ξ is a parameter describing limit value of the phase transition velocity [4], and k is a positive kinetic factor. Equation (27) with (28) can be considered as the special constitutive equation describing motion of phase interfaces in shells.

Summarising, in the case of finite deformations the non-linear thermomechanic BVP for thermoelastic or thermoviscoelastic shells undergoing phase transition consists of:

- the equilibrium equations $(8)_1$ supplemented by appropriate static and kinematic boundary conditions for N , M , u , and Q ,
- the thermoconductivity equations (12) and (13) with appropriate boundary conditions for θ and φ ,
- \bullet the compatibility conditions (20), (21), and (24) along the interface *C*,
- the kinetic equation (27) along *C*,

all supplemented with proper constitutive equations for *N*, *M*, ε , η , χ , q , and *s*, see [10]. The kinetic equation (27) is used to find position of the curvilinear interface *C* in its quasistatic motion.

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