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Dedicated to the memory of Professor Pavel Zhilin

The non-linear theory of elastic shells undergoing phase transitions was proposed by two first authors in J. Elast. **79**, 67–86 (2004). In the present paper the theory is extended by taking into account also the elastic strain energy density of the curvilinear phase interface as well as the resultant forces and couples acting along the interface surface curve itself. All shell relations are found from the variational principle of stationary total potential energy. In particular, we derive the extended natural continuity conditions at coherent and/or incoherent surface curves modelling the phase interface. The continuity conditions allow one to establish the final position of the interface surface curve after the phase transition. The results are illustrated by an example of a phase transition in an infinite plate with a central hole.

1 Introduction

The non-linear mechanical theory of elastic shells with an account of occurence of the martensitic type phase transition (PT) in the material was developed by Eremeyev and Pietraszkiewicz [1]. The formulation was based on the dynamically and kinematically exact shell model [2–4] with displacements composed of work-averaged translations and rotations of the shell cross sections. Such a general shell model had a structure of the classical Cosserat surface [5] to which Professor Pavel Zhilin contributed in [6–8]. In particular, in [1] we derived new static natural continuity conditions at the curvilinear phase interface. To model the phase equilibrium we used in [1] the variational approach based on the Gibbs variational principle [9]. Variational methods in the theory of phase transitions were developed in many papers and books, see for example [10–12].

Within 3D theories of phase transformation phenomena the phase interface is usually modelled by a sharp smoothly evolving surface separating different material phases in the thermodynamic equilibrium state. The surface interface itself may be endowed with various additional fields modelling different types of PTs, see for example Grinfeld [10] and Podstrigach and Povstenko [13], where many references are given. In particular, Povstenko [14] reviewed various models of the surface interfaces and three-phase line interface junctions in 3D continuum and proposed to treat them as 2D and 1D continua of the Cosserat type, respectively. Within 2D theories of thin films and biomembranes undergoing PTs simple 1D models of the interface surface curve were discussed by Wang [15], Atai and Steigmann [16], Boulbitch [17], Bhattacharya and James [18], Shu [19], James and Rizzoni [20], Roytburd and Slutsker [21], Gurtin and Jabbour [22], and Rubin et al. [23]. However, neither of those 1D models is complete enough to be applied with the non-linear theory of shells with PTs developed in [1]. The model of PTs in martensitic films developed in [18–20] was based on the Cosserat-type membrane theory which is a special case of the theory of shells. In [1] we proposed the most general model of such thin-walled bodies undergoing PTs. Our formulation of shell theory is based on the statically and kinematically exact through-the-thickness reduction of three-dimensional description of the phenomenon to two-dimensional form written on the shell base surface [1–4]. Using the general theory of shells we can describe the stress-induced PTs taking into account not only the tangentional stiffness but also the bending as well as transverse shear and normal stiffnesses of such martensitic films.

The aim of this paper is to extend the results of [1] by taking into account also the elastic strain energy density of the phase interface itself as well as additional resultant forces and couples acting along the interface surface curve and at its intersections with the shell boundary contour. The curvilinear density allows one to model within shell theory also

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generalized capillary type phenomena widely discussed in continuum mechanics with PT, [10,13]. The additional forces and couples along the curvilinear interface may appear as a result of exact reduction to 1D problem of the 3D PT phenomenon in a thin tube about the interface surface curve, as it is given for branching and self-intersecting shells in [24,25].

After reviewing the kinematic relations in Sect. 2, the equilibrium problem of PTs in elastic shells is formulated in Sect. 3 in the weak form as the stationary problem for the functional of total potential energy (7). Stationarity conditions of the functional following from (11) give the local equilibrium equations and static natural boundary conditions known from [1–4]. Along the curvilinear interface we obtain the new, local, natural continuity conditions (13), (14) which extend those proposed in [1]. The latter conditions allow one to establish position of the interface curve in the thermodynamic equilibrium state of PT in shells. Coherent curvilinear interfaces and interfaces incoherent in rotations are discussed in more detail in Subsections 4.1 and 4.2, respectively, where specific results appropriate to those two cases are given. The extended theory of PTs in shells is illustrated by a simple example of an infinite plate with a central hole discussed in [1], but now endowed with an additional capillary tension along the interface circle.

2 Kinematic relations

Within the dynamically and kinematically exact theory of regular shells [2–4], a shell is a three-dimensional (3D) solid body identified in a reference (undeformed) placement κ with a region B of the physical space $\mathcal{E}$ having the 3D vector space E as its translation space. Geometry of B is described in the normal coordinates (θ^α, ξ), $\alpha = 1, 2$, where $\xi = 0$ defines the regular base surface $M \subset B$, and $\xi \in \left[-h^-, h^+\right]$ is the distance from M, with $h = h^- + h^+$ the shell thickness. If $\boldsymbol{x} \in E$ is the position vector of $x \in M$, then the surface covariant and contravariant base vectors $\boldsymbol{a}_\alpha$ and $\boldsymbol{a}^\beta$ are defined by

$$\boldsymbol{a}_\alpha = \frac{\partial \boldsymbol{x}}{\partial \theta^\alpha} \equiv \boldsymbol{x}_{,\alpha} \,, \quad \boldsymbol{a}^\beta \cdot \boldsymbol{a}_\alpha = \delta_\alpha^\beta \,, \quad \boldsymbol{\eta} = \frac{1}{2} \epsilon^{\alpha\beta} \boldsymbol{a}_\alpha \times \boldsymbol{a}_\beta \,, \tag{1}$$

where $\boldsymbol{\eta}$ is the unit normal orienting M and $\epsilon^{\alpha\beta}$ are contravariant components of the surface permutation tensor $\boldsymbol{\epsilon}$.

In the deformed placement γ the shell can be represented by the position vector $\boldsymbol{y} = \chi(\boldsymbol{x}) \in E$ of the material base surface $N = \chi(M)$ with attached three directors $\boldsymbol{d}_\alpha, \boldsymbol{d}$ such that

$$\boldsymbol{y} = \boldsymbol{x} + \boldsymbol{u} \,, \quad \boldsymbol{d}_\alpha = \boldsymbol{Q}\boldsymbol{a}_\alpha \,, \quad \boldsymbol{d} = \boldsymbol{Q}\boldsymbol{\eta} \,, \tag{2}$$

where χ is the deformation function, while $\boldsymbol{u} \in E$ is the translation vector of M and $\boldsymbol{Q} \in SO(3)$ the proper orthogonal (rotation) tensor, $\boldsymbol{Q}^T = \boldsymbol{Q}^{-1}$, $\det \boldsymbol{Q} = +1$, describing the work-averaged gross deformation of the shell cross section.

The shell strain and bending tensors $\boldsymbol{E}$ and $\boldsymbol{K}$ in the spatial representation can be defined by [1–3]

$$\boldsymbol{E} = \boldsymbol{\varepsilon}_\alpha \otimes \boldsymbol{a}^\alpha \,, \quad \boldsymbol{K} = \boldsymbol{\kappa}_\alpha \otimes \boldsymbol{a}^\alpha \,,$$

$$\boldsymbol{\varepsilon}_\alpha = \boldsymbol{y}_{,\alpha} - \boldsymbol{d}_\alpha = \boldsymbol{u}_{,\alpha} + (\boldsymbol{1} - \boldsymbol{Q})\, \boldsymbol{a}_\alpha = E_{\alpha\beta} \boldsymbol{d}^\beta + E_\alpha \boldsymbol{d} \,,$$

$$\boldsymbol{\kappa}_\alpha = ax\left(\boldsymbol{Q}_{,\alpha}\boldsymbol{Q}^T\right) = \frac{1}{2}\left\{\boldsymbol{d}^\beta \times \left(\boldsymbol{Q}_{,\alpha}\boldsymbol{Q}^T\right)\boldsymbol{d}_\beta + \boldsymbol{d} \times \left(\boldsymbol{Q}_{,\alpha}\boldsymbol{Q}^T\right)\boldsymbol{d}\right\} = \boldsymbol{d} \times K_{\alpha\beta}\boldsymbol{d}^\beta + K_\alpha \boldsymbol{d} \,. \tag{3}$$

In a two-phase elastic shell different material phases may appear in different complementary subregions N_A and N_B of N separated by the curvilinear phase interface $D \in N$, Fig.1. For a continuous deformation χ we can introduce on M a singular image curve $C = \chi^{-1}(D)$ separating the corresponding image regions $M_A = \chi^{-1}(N_A)$ and $M_B = \chi^{-1}(N_B)$. The position vectors of C and D are related by $\boldsymbol{x}_C(s) = \chi^{-1}\left(\boldsymbol{y}_C(s)\right)$, where s is the arc length parameter along C.

The equilibrium boundary value problem (BVP) for shells with PTs was formulated in [1] in the weak form as the stationary problem for the functional of total potential energy. In the functional of [1] we did not take into account physical properties of the curvilinear interface itself such as, for example, the line tension of capillarity type and its possible generalizations. Also force and couple resultants acting along C and at its intersections with ∂M were not accounted for in [1]. To extend the functional of [1] by additional effects associated with C let us remind some kinematical relations of the surface curve C treated here as an axis of a virtual rod.

Within the dynamically and kinematically exact theory of regular rods developed in [3,26] the initial (undeformed) placement κ of the 3D rod-like body is represented by the position vector $\boldsymbol{x}_C \in E$ of the axis C and three orthonormal vectors $\boldsymbol{\tau}_\alpha, \boldsymbol{\tau}$ attached to any point $x_C \in C$, with $\boldsymbol{\tau} = d\boldsymbol{x}_C/ds \equiv \boldsymbol{x}_C'$. In the deformed placement γ the rod is represented by the position vector $\boldsymbol{y}_C \in E$ of the material rod axis $D = \chi(C)$ and three attached orthonormal directors $\boldsymbol{h}_\alpha, \boldsymbol{h}$ which satisfy the relations

$$\boldsymbol{y}_C = \chi(\boldsymbol{x}_C) = \boldsymbol{x}_C + \boldsymbol{u}_C \,, \quad \boldsymbol{h}_\alpha = \boldsymbol{R}\boldsymbol{\tau}_\alpha \,, \quad \boldsymbol{h} = \boldsymbol{R}\boldsymbol{\tau} \,, \tag{4}$$
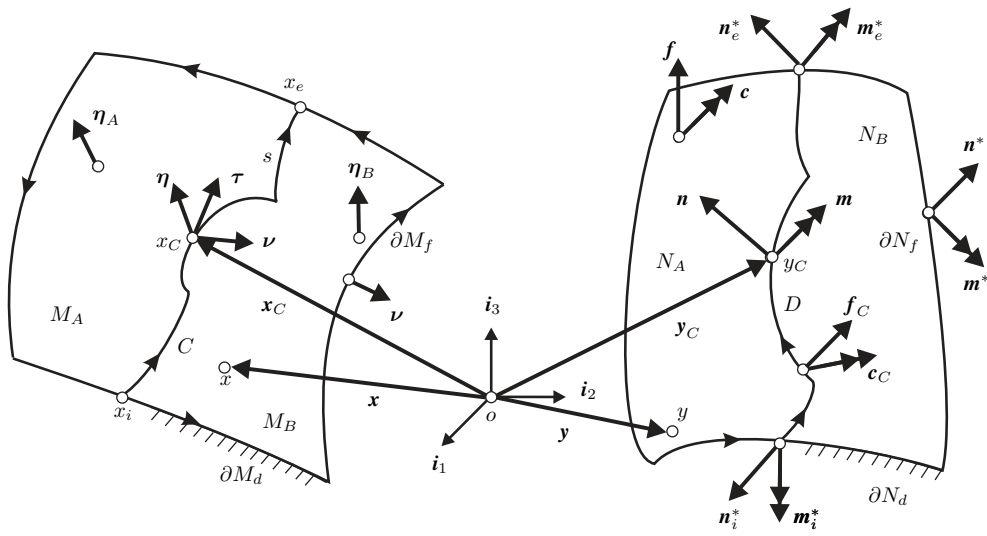
Fig. 1 Two-phase shell kinematics.

where $\boldsymbol{u}_C$ is the translation vector and $\boldsymbol{R}$ the rotation tensor describing the work-averaged gross deformation of the rod cross section.

The local deformation of the phase interface curve C can be described by the natural strain $\boldsymbol{\varepsilon}$ and bending $\boldsymbol{\kappa}$ vectors in the spatial representation defined by [3, 26]

$$\boldsymbol{\varepsilon} = \boldsymbol{u}'_C + (\boldsymbol{1} - \boldsymbol{R})\,\boldsymbol{\tau}\,,\quad \boldsymbol{\kappa} = ax\left(\boldsymbol{R}'\boldsymbol{R}^T\right)\,. \tag{5}$$

The 1D fields $\boldsymbol{u}_C(s), \boldsymbol{R}(s)$ along C can be different, in general, from finite limits $\boldsymbol{u}^{\pm}(s), \boldsymbol{Q}^{\pm}(s)$ of the 2D fields $\boldsymbol{u}, \boldsymbol{Q}$ when the respective boundaries ∂M_A or ∂M_B coinciding with C are approached. As a result, each type of the phase transition should be characterised by additional relations between $\boldsymbol{u}_C, \boldsymbol{R}$ and $\boldsymbol{u}^{\pm}, \boldsymbol{Q}^{\pm}$. 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 C is called *coherent* if both fields $\boldsymbol{y}$ and $\boldsymbol{Q}$ are continuous at C

$$\boldsymbol{y}^- = \boldsymbol{y}^+ = \boldsymbol{y}_C\,,\quad [\![\,\boldsymbol{y}\,]\!] = \boldsymbol{0}\,,\quad [\![\,\boldsymbol{y}'\,]\!] = \boldsymbol{0}\,,$$

$$\boldsymbol{Q}^- = \boldsymbol{Q}^+ = \boldsymbol{R}\,,\quad [\![\,\boldsymbol{Q}\,]\!] = \boldsymbol{0}\,,\quad [\![\,\boldsymbol{Q}'\,]\!] = \boldsymbol{0}\,, \tag{6}$$

where $[\![\,...\,]\!] = (...)^+ - (...)^-$ is the jump at C. Therefore, the coherent curve C can be singular with regard to $\boldsymbol{F} = Grad_s\boldsymbol{y}$ and $Grad_s\boldsymbol{Q}$ but not with regard to $\boldsymbol{y}$ and $\boldsymbol{Q}$ themselves, where $Grad_s$ is the surface gradient operator defined intrinsically in [27, 28].

The phase interface is called *incoherent in rotations* if $\boldsymbol{y}$ is continuous at C but continuity of $\boldsymbol{Q}$ at C is violated. In this case the conditions indicated in the first row of (6) are still satisfied, but those indicated in the second row of (6) can be violated. Therefore, the interface C incoherent in rotations can be singular with regard to $\boldsymbol{F}$, $Grad_s\boldsymbol{Q}$, and $\boldsymbol{Q}$.

3 Weak formulation of equilibrium BVP

The equilibrium BVP for shells with occurrence of the PT can now be formulated in the following weak form extending the one proposed in [1, 29]:

Given the external, resultant surface force and couple fields $\boldsymbol{f}(\theta^\alpha), \boldsymbol{c}(\theta^\alpha)$ on M, curvilinear force and couple fields $\boldsymbol{f}_C(s)$, $\boldsymbol{c}_C(s)$ along C, concentrated forces and couples $\boldsymbol{n}_i^*, \boldsymbol{m}_i^*$ and $\boldsymbol{n}_e^*, \boldsymbol{m}_e^*$ acting at initial and end points x_i, x_e of intersection of C with ∂M_f, as well as boundary force and couple fields $\boldsymbol{n}^*(s), \boldsymbol{m}^*(s)$ prescribed along ∂M_f, respectively, find a solution $(\boldsymbol{u}, \boldsymbol{Q}, \boldsymbol{x}_C)$ on the configuration space $S\left(M; E \times SO(3) \times E\right)$ 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 vector fields $\delta\boldsymbol{u}, \boldsymbol{w} = ax\left(\delta\boldsymbol{Q}\boldsymbol{Q}^T\right), \delta\boldsymbol{x}_C$ the following variational principle of the total potential energy is satisfied:

$$\delta I = 0\,,\quad I = \iint_{M_A} W_A\,\mathrm{d}a + \iint_{M_B} W_B\,\mathrm{d}a + \int_C W_C\,\mathrm{d}s - A\,. \tag{7}$$

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, respectively, $W_C = W_C(\varepsilon, \boldsymbol{\kappa})$ is the 1D elastic strain energy density associated with the phase interface curve C, and A is the potential of external loads such that

$$
\delta A = \iint_{M \setminus C} (\boldsymbol{f} \cdot \delta \boldsymbol{u} + \boldsymbol{c} \cdot \boldsymbol{w}) \, \mathrm{d}a + \int_C (\boldsymbol{f}_C \cdot \delta \boldsymbol{u}_C + \boldsymbol{c}_C \cdot \boldsymbol{w}_C) \, \mathrm{d}s
$$

$$
+ \int_{\partial M_f} (\boldsymbol{n}^* \cdot \delta \boldsymbol{u} + \boldsymbol{m}^* \cdot \boldsymbol{w}) \, \mathrm{d}s + \boldsymbol{n}_e^* \cdot \delta \boldsymbol{u}_e + \boldsymbol{m}_e^* \cdot \boldsymbol{w}_e - \boldsymbol{n}_i^* \cdot \delta \boldsymbol{u}_i - \boldsymbol{m}_i^* \cdot \boldsymbol{w}_i . \tag{8}
$$

In (8), $\delta \boldsymbol{u}_C$ and $\boldsymbol{w}_C = ax(\delta \boldsymbol{R} \boldsymbol{R}^T)$ are the virtual translation and rotation of the interface C, and corresponding virtual displacements at the initial and end points of C are denoted by $\delta \boldsymbol{u}_i$, $\boldsymbol{w}_i$ and $\delta \boldsymbol{u}_e$, $\boldsymbol{w}_e$, respectively.

The principle $(7)_1$ with $(7)_2$ and (8) states that among all possible values of $\boldsymbol{u}, \boldsymbol{Q}$ in $M \setminus C$, $\boldsymbol{u}_C, \boldsymbol{R}$ along C, and positions of the phase interface $\boldsymbol{x}_C$ the actual solution renders the functional $(7)_2$ stationary.

Calculating δI with I defined by $(7)_2$ consists of two parts. In the first part we have to repeat all transformations given in detail in [1] for I without the integral over C in $(7)_2$ as well as without the integral over C and out of integral terms in (8). Due to the limited volume of this paper we do not repeat here those transformations and refer the reader to the final result given in [1], f. (26).

Variation of the additional integral in $(7)_2$ performed with the help of (5) and the theorem for differentiation of curvilinear integrals [13] (f. (1.158), (2.223)) or [30] (f. 24) with a movable surface curve leads to

$$
\delta \int_C W_C \, \mathrm{d}s = \int_C \delta W_C \mathrm{d}s + \int_C k_g V W_C \mathrm{d}s
$$

$$
= \int_C (\boldsymbol{n} \cdot \delta^c \varepsilon + \boldsymbol{m} \cdot \delta^c \boldsymbol{\kappa}) \, \mathrm{d}s + \int_C k_g V W_C \mathrm{d}s
$$

$$
= \int_C \left\{ \boldsymbol{n} \cdot (\delta \boldsymbol{u}_C' - \boldsymbol{w}_C \times \boldsymbol{y}_C') + \boldsymbol{m} \cdot \boldsymbol{w}_C' \right\} \, \mathrm{d}s + \int_C k_g V W_C \mathrm{d}s
$$

$$
= (\boldsymbol{n} \cdot \delta \boldsymbol{u}_C + \boldsymbol{m} \cdot \boldsymbol{w}_C) \big|_{x_i}^{x_e} - \int_C \left\{ \boldsymbol{n}' \cdot \delta \boldsymbol{u}_C + (\boldsymbol{m}' + \boldsymbol{y}_C' \times \boldsymbol{n}) \cdot \boldsymbol{w}_C \right\} \mathrm{d}s + \int_C k_g V W_C \mathrm{d}s , \tag{9}
$$

where δ^c is the corotational variation, $k_g = -\dfrac{\partial \boldsymbol{\tau}}{\partial s} \cdot \boldsymbol{\nu}$ is the geodesic curvature of C, $\boldsymbol{\nu}$ is the external unit normal to ∂M, $V = \delta \boldsymbol{x}_C \cdot \boldsymbol{\nu}$, and we have used the relations for $\delta^c \varepsilon$ and $\delta^c \boldsymbol{\kappa}$ given in [3]. Because we are interested in the continuity conditions along C we assume here that $\delta \boldsymbol{x}_C = \boldsymbol{0}$ at the end points of C to avoid discussion of the continuity conditions at the singular points which we feel to be of secondary importance in this problem. We may also consider the closed curve C. The stress resultant $\boldsymbol{n}$ and stress couple $\boldsymbol{m}$ vectors in the spatial representation are given by the constitutive equations

$$
\boldsymbol{n} = \frac{\partial W_C}{\partial \varepsilon} , \quad \boldsymbol{m} = \frac{\partial W_C}{\partial \boldsymbol{\kappa}} . \tag{10}
$$

Introducing (9) and (8) into $(7)_1$ and using the results of transformations given in [1], f. (26) we obtain

$$
\delta I = - \iint_{M \setminus C} \left\{ \left(\boldsymbol{n}^\alpha \big|_\alpha + \boldsymbol{f} \right) \cdot \delta \boldsymbol{u} + \left(\boldsymbol{m}^\alpha \big|_\alpha + \boldsymbol{y}_{,\alpha} \times \boldsymbol{n}^\alpha + \boldsymbol{c} \right) \cdot \boldsymbol{w} \right\} \mathrm{d}a
$$

$$
+ \int_{\partial M_f} \left\{ (\boldsymbol{n}_\nu - \boldsymbol{n}^*) \cdot \delta \boldsymbol{u} + (\boldsymbol{m}_\nu - \boldsymbol{m}^*) \cdot \boldsymbol{w} \right\} \mathrm{d}s
$$

$$
+ \int_{\partial M_d} (\boldsymbol{n}_\nu \cdot \delta \boldsymbol{u} + \boldsymbol{m}_\nu \cdot \boldsymbol{w}) \, \mathrm{d}s
$$

$$
- \int_C \left\{ V [\![W]\!] - k_g V W_C + [\![\boldsymbol{n}_\nu \cdot \delta \boldsymbol{u}]\!] + [\![\boldsymbol{m}_\nu \cdot \boldsymbol{w}]\!] \right.
$$

$$
+ \left. (\boldsymbol{n}' + \boldsymbol{f}_C) \cdot \delta \boldsymbol{u}_C + (\boldsymbol{m}' + \boldsymbol{y}_C' \times \boldsymbol{n} + \boldsymbol{c}_C) \cdot \boldsymbol{w}_C \right\} \mathrm{d}s
$$

$$
+ (\boldsymbol{n}_e - \boldsymbol{n}_e^*) \cdot \delta \boldsymbol{u}_e + (\boldsymbol{m}_e - \boldsymbol{m}_e^*) \cdot \boldsymbol{w}_e - (\boldsymbol{n}_i - \boldsymbol{n}_i^*) \cdot \delta \boldsymbol{u}_i - (\boldsymbol{m}_i - \boldsymbol{m}_i^*) \cdot \boldsymbol{w}_i = 0 , \tag{11}
$$

where

$$n^\alpha = \frac{\partial W}{\partial \boldsymbol{\varepsilon}_\alpha} \,, \quad m^\alpha = \frac{\partial W}{\partial \boldsymbol{\kappa}_\alpha} \,, \quad \boldsymbol{n}_\nu = N\boldsymbol{\nu} = \boldsymbol{n}^\alpha \nu_\alpha \,, \quad \boldsymbol{m}_\nu = M\boldsymbol{\nu} = \boldsymbol{m}^\alpha \nu_\alpha \,, \tag{12}$$

$\nu_\alpha = \boldsymbol{\nu} \cdot \boldsymbol{a}_\alpha$, and N, M are the stress resultant and stress couple tensors of the Kirchhoff type, respectively.

Vanishing of the first two rows of (11) leads to known local equilibrium equations and natural boundary conditions of the general theory of regular shells, see [1]. The third and sixth rows of (11) vanish identically if the kinematic boundary conditions along ∂M_d are satisfied, for then $\delta\boldsymbol{u} = \boldsymbol{w} = \delta\boldsymbol{u}_e = \boldsymbol{w}_e = \delta\boldsymbol{u}_i = \boldsymbol{w}_i = \boldsymbol{0}$ along ∂M_d.

4 Extended natural continuity conditions

From (11) it also follows that at the curvilinear phase interface the following local, extended, static natural continuity conditions have to be satisfied:

$$V[\![\,W\,]\!] - k_g V W_C + [\![\,\boldsymbol{n}_\nu \cdot \delta\boldsymbol{u}\,]\!] + [\![\,\boldsymbol{m}_\nu \cdot \boldsymbol{w}\,]\!] + (\boldsymbol{n}' + \boldsymbol{f}_C) \cdot \delta\boldsymbol{u}_C + (\boldsymbol{m}' + \boldsymbol{y}'_C \times \boldsymbol{n} + \boldsymbol{c}_C) \cdot \boldsymbol{w}_C = 0 \quad \text{along } C, \tag{13}$$

$$\boldsymbol{n}_i = \boldsymbol{n}_i^* \,, \quad \boldsymbol{m}_i = \boldsymbol{m}_i^* \quad \text{at } x_i = C \cap \partial M_f \,,$$

$$\boldsymbol{n}_e = \boldsymbol{n}_e^* \,, \quad \boldsymbol{m}_e = \boldsymbol{m}_e^* \quad \text{at } x_e = C \cap \partial M_f \,. \tag{14}$$

The fields V, $\delta\boldsymbol{u}^\pm$, $\boldsymbol{w}^\pm$, $\delta\boldsymbol{u}_C$, $\boldsymbol{w}_C$ in (13) are still not independent at C, in general. Performing more detailed analysis of (13) for different types of PTs we can introduce additional information about the behavior of the virtual fields and their interrelation.

Assuming that $\boldsymbol{y}(x)$ and $\boldsymbol{Q}(x)$ are smooth fields in the interiors of M_A and M_B we can define one-sided limits $\boldsymbol{y}^\pm$, $\boldsymbol{F}^\pm$, $\boldsymbol{Q}^\pm$, $(Grad_s\boldsymbol{Q})^\pm$ when $x \to x_C$. The functions $\boldsymbol{y}^\pm(s)$ and $\boldsymbol{Q}^\pm(s)$ are continuously differentiable along C.

4.1 Coherent interface

For the coherent interface all the relations (6) are assumed to be satisfied. Then applying the Maxwell theorem [31] we obtain the local kinematic compatibility conditions [1]

$$[\![\,\delta\boldsymbol{u}\,]\!] + V[\![\,\boldsymbol{F}\boldsymbol{\nu}\,]\!] = \boldsymbol{0}\,, \quad [\![\,\boldsymbol{w}\,]\!] + V[\![\,\boldsymbol{K}\boldsymbol{\nu}\,]\!] = \boldsymbol{0} \quad \text{along } C \,, \tag{15}$$

$$\boldsymbol{F}\boldsymbol{\nu} = \boldsymbol{y}_{,\alpha}\,\nu^\alpha \,, \quad \boldsymbol{K}\boldsymbol{\nu} = \boldsymbol{\kappa}_\alpha \nu^\alpha \,, \tag{16}$$

which allow one to relate $[\![\,\delta\boldsymbol{u}\,]\!]$ and $[\![\,\boldsymbol{w}\,]\!]$ with V.

Let us represent the jumps of products in (13) by the identities

$$[\![\,N\boldsymbol{\nu} \cdot \delta\boldsymbol{u}\,]\!] = \langle N\boldsymbol{\nu}\rangle \cdot [\![\,\delta\boldsymbol{u}\,]\!] + [\![\,N\boldsymbol{\nu}\,]\!] \cdot \langle\delta\boldsymbol{u}\rangle \,, \quad [\![\,M\boldsymbol{\nu} \cdot \boldsymbol{w}\,]\!] = \langle M\boldsymbol{\nu}\rangle \cdot [\![\,\boldsymbol{w}\,]\!] + [\![\,M\boldsymbol{\nu}\,]\!] \cdot \langle\boldsymbol{w}\rangle \,. \tag{17}$$

Introducing (15) and (17) into (13) we obtain

$$V\left\{[\![\,W\,]\!] - k_g W_C - \langle N\boldsymbol{\nu}\rangle \cdot [\![\,\boldsymbol{F}\boldsymbol{\nu}\,]\!] - \langle M\boldsymbol{\nu}\rangle \cdot [\![\,\boldsymbol{K}\boldsymbol{\nu}\,]\!]\right\} + [\![\,N\boldsymbol{\nu}\,]\!] \cdot \langle\delta\boldsymbol{u}\rangle + [\![\,M\boldsymbol{\nu}\,]\!] \cdot \langle\boldsymbol{w}\rangle$$
$$+ (\boldsymbol{n}' + \boldsymbol{f}_C) \cdot \delta\boldsymbol{u}_C + (\boldsymbol{m}' + \boldsymbol{y}'_C \times \boldsymbol{n} + \boldsymbol{c}_C) \cdot \boldsymbol{w}_C = 0 \,. \tag{18}$$

At the coherent interface C from (6) it follows that $\langle\delta\boldsymbol{u}\rangle = \delta\boldsymbol{u}_C$ and $\langle\boldsymbol{w}\rangle = \boldsymbol{w}_C$. Therefore

$$V\left\{[\![\,W\,]\!] - k_g W_C - \langle N\boldsymbol{\nu}\rangle \cdot [\![\,\boldsymbol{F}\boldsymbol{\nu}\,]\!] - \langle M\boldsymbol{\nu}\rangle \cdot [\![\,\boldsymbol{K}\boldsymbol{\nu}\,]\!]\right\}$$
$$+ (\boldsymbol{n}' + [\![\,N\boldsymbol{\nu}\,]\!] + \boldsymbol{f}_C) \cdot \delta\boldsymbol{u}_C + (\boldsymbol{m}' + \boldsymbol{y}'_C \times \boldsymbol{n} + [\![\,M\boldsymbol{\nu}\,]\!] + \boldsymbol{c}_C) \cdot \boldsymbol{w}_C = 0 \,. \tag{19}$$

For now independent virtual fields V, $\delta\boldsymbol{u}_C$, and $\boldsymbol{w}_C$ the relation (19) requires that the following local continuity conditions be satisfied along C:

$$[\![\,W\,]\!] - \langle N\boldsymbol{\nu}\rangle \cdot [\![\,\boldsymbol{F}\boldsymbol{\nu}\,]\!] - \langle M\boldsymbol{\nu}\rangle \cdot [\![\,\boldsymbol{K}\boldsymbol{\nu}\,]\!] = k_g W_C \,,$$

$$\boldsymbol{n}' + [\![\,N\boldsymbol{\nu}\,]\!] + \boldsymbol{f}_C = \boldsymbol{0}\,, \quad \boldsymbol{m}' + \boldsymbol{y}'_C \times \boldsymbol{n} + [\![\,M\boldsymbol{\nu}\,]\!] + \boldsymbol{c}_C = \boldsymbol{0} \,. \tag{20}$$

The continuity conditions (14) and (20) are more complex than those derived in [1], f. $(37)_{1,2}$ and (39), because now they bring additional information about the elastic strain energy associated with the phase interface itself as well as the resultant forces and couples acting along C and at the initial x_i and end x_e points of C. The conditions (14) and $(20)_{2,3}$ are formally the same as the ones of the exact, resultant, static continuity conditions of the branching and intersecting shells [25] derived by direct through-the-thickness integration of equilibrium conditions of continuum mechanics. This suggests that the conditions (14) and (20) can also be formulated exactly by direct through-the-thickness integration of appropriate 3D equilibrium conditions of the shell-like body undergoing PT in a thin tube of matter about the singular surface curve C.

4.2 Interface incoherent in rotations

For the interface incoherent in rotations only the relations of the first row of (6) are assumed to be satisfied. In this case the interface C can be singular with regard to Q, F, and $Grad_sQ$. From the Maxwell theorem [31] follows only the first compatibility condition $(6)_1$, while the second one $(6)_2$ can now be violated, in general. Here $\langle\delta\mathbf{u}\rangle = \delta\mathbf{u}_C$ as well, but $\langle w\rangle \neq w_C$, in general. Then the continuity condition (13) can be transformed into

$$V\left\{[\![\, W \,]\!] - k_g W_C - \langle N\nu\rangle \cdot [\![\, F\nu \,]\!]\right\} + [\![\, M\nu \cdot w \,]\!]$$
$$+ \left(n' + [\![\, N\nu \,]\!] + f_C\right)\cdot \delta u_C + \left(m' + y'_C \times n + c_C\right)\cdot w_C = 0. \tag{21}$$

With now independent virtual fields V, $w^\pm$, δu_C, w_C the relation (21) is equivalent to the following set of local, static, natural continuity conditions along the interface C incoherent in rotations:

$$[\![\, W \,]\!] - \langle N\nu\rangle \cdot [\![\, F\nu \,]\!] = k_g W_C, \quad M^\pm\nu = 0,$$
$$n' + [\![\, N\nu \,]\!] + f_C = 0, \quad m' + y'_C \times n + c_C = 0. \tag{22}$$

The second conditions in the first row of (22) indicate that here there appears the kind of a hinge along C at which the resultant surface couples should vanish. The conditions (22) express just the balance of forces and couples at the interface C incoherent in rotations.

The static natural continuity conditions $(20)_1$ and $(22)_1$ are the relations which allow one to establish position of the singular curve C on M in the thermodynamic equilibrium state of phase transition.

4.3 Capillary energy of the phase interface

Let us consider a special case of curvilinear energy of the phase interface by analogy to the one used in the theory of capillary surfaces [32, 33]. In our 1D case the therm responsible for curvilinear energy in the functional (7) can be assumed to be given by the integral along D

$$\sigma \int_D \mathrm{d}\bar{s}, \quad \text{where } \mathrm{d}\bar{s} = \sqrt{y'_C \cdot y'_C}\,\mathrm{d}s, \text{ therefore } W_C = \sigma\sqrt{y'_C \cdot y'_C}. \tag{23}$$

Here σ is the constant line tension, while $\bar{s}$ is the length parameter along D. Other possible types of constitutive equations of one-dimensional continua are discussed in [13]. 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 describes the energy of a tube surrounding the dislocation, see [34]. For the curvilinear energy (23) we can simplify the continuity conditions along the phase interface (20) and (22). Indeed, if we use (10) then from the equation (23) we obtain

$$n = \frac{\sigma}{\sqrt{y'_C \cdot y'_C}}y'_C, \quad m = 0. \tag{24}$$

Thus, using (24) we obtain that $n \times y'_C = 0$. If we further assume that $c_C = 0$ the third equation of (20) reduces to $[\![\, M\nu \,]\!] = 0$ while the fourth one of (22) is satisfied identically.

Note that $\frac{1}{\sqrt{y'_C \cdot y'_C}}y'_C$ is the unit vector tangent to the curve D. Then using the Frenet formulas we obtain that $\left(\frac{1}{\sqrt{y'_C \cdot y'_C}}y'_C\right)' = k\mu$, where k is the principal curvature of the curve D and μ is the principal unit normal to D. Then with the additional assumption that $f_C = 0$ the second equation of (20) or the third one of (22) reduces to

$$\sigma k\mu + [\![\, N\nu \,]\!] = 0. \tag{25}$$

The equation (25) is a 1D analog of the well-known Laplace equation in the theory of capillarity [32, 33].

5 Example

Let us solve a simple axisymmetric plane problem of PT in an infinite plate with a central hole of radius a taking into account the curvilinear energy given by (23), Fig. 2. This example was considered in [1] in the case $\sigma = 0$. It is assumed that in
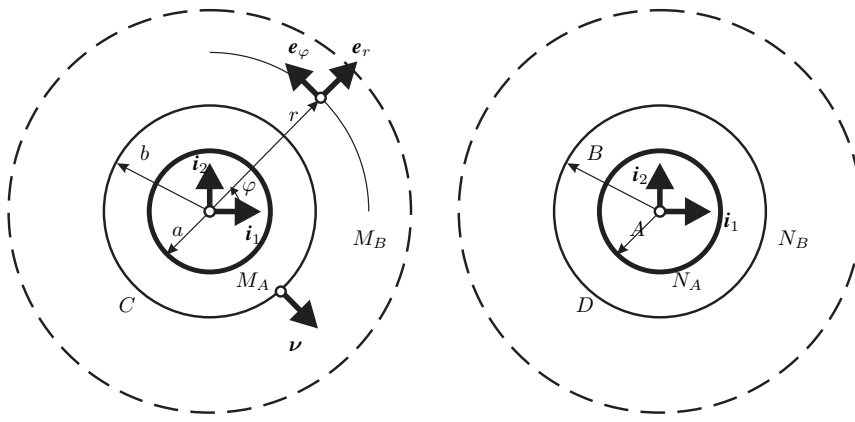
Fig. 2 Two-phase plate with a hole.

the undeformed state the whole plate consists of one material phase marked by "B". Then to the hole boundary the radial translation $\boldsymbol{u}^* = -u^* \, \boldsymbol{e}_r$ with a constant magnitude u^* is prescribed. As a result, in the deformed equilibrium state of phase transition there may appear in a region $a < r < b$ a new material phase marked by "A". Our goal is to find the radius b of the interface circle C.

In the polar coordinate system $\theta^1 = r, \theta^2 = \varphi$ the axisymmetric plane deformation and corresponding strain and bending measures are given by

$$
\begin{aligned}
&\boldsymbol{y} = y(r)\boldsymbol{e}_r, \quad \boldsymbol{u} = u(r)\boldsymbol{e}_r = (y(r) - r)\boldsymbol{e}_r, \quad \boldsymbol{Q} = \boldsymbol{1}, \quad \boldsymbol{y}_C = B\boldsymbol{e}_r, \quad \boldsymbol{x}_C = b\boldsymbol{e}_r, \\
&\boldsymbol{e}_r = \cos\varphi\boldsymbol{i}_1 + \sin\varphi\boldsymbol{i}_2, \quad \boldsymbol{e}_\varphi = -\sin\varphi\boldsymbol{i}_1 + \cos\varphi\boldsymbol{i}_2, \\
&\boldsymbol{\varepsilon}_r = \frac{du}{dr}\boldsymbol{e}_r \equiv u' \, \boldsymbol{e}_r, \quad \boldsymbol{\varepsilon}_\varphi = u\boldsymbol{e}_\varphi, \quad \boldsymbol{\kappa}_r = \boldsymbol{\kappa}_\varphi \equiv \boldsymbol{0}, \\
&\boldsymbol{E} = E_r\boldsymbol{e}_r \otimes \boldsymbol{e}_r + E_\varphi\boldsymbol{e}_\varphi \otimes \boldsymbol{e}_\varphi, \quad E_r = u', \quad E_\varphi = \frac{u}{r},
\end{aligned}
\tag{26}
$$

where $\boldsymbol{e}_r$ and $\boldsymbol{e}_\varphi$ are the unit base vectors, E_r and E_φ are the physical components of strain, while B or b and $y(r)$ or $u(r)$ are unknowns of the BVP.

To avoid awkward computations of [1] the elastic strain energy densities W_A and W_B are assumed in the simple form

$$
W_{A,B} = C_1^{A,B} \left(E_r^2 + E_\varphi^2 \right) + \Delta_{A,B} \equiv C_1^{A,B} \left(u'^2 + \frac{u^2}{r^2} \right) + \Delta_{A,B},
\tag{27}
$$

where $\Delta_{A,B}$ is a constant. Usually we determine the strain energy density with accuracy to a constant, but here we may take into account that the reference values of the densities of the two phases at zero strains may be different, in general. If we assume that $\Delta_B = 0$, then Δ_A describes an energetic barrier for the formation of the new phase "A". Further we take $\Delta_A \equiv C_1^A \Delta \neq 0$ where Δ is a dimensionless parameter. The one-constant constitutive equation (27) means that the strain energy densities of two material phases differ only by values of elastic constants $C_1^{A,B}$ while other elastic constants in the constitutive equation of isotropic shell discussed in [1] are equal zero.

For the deformation (26) and the constitutive equations (24) and (27) we have

$$
\begin{aligned}
&\boldsymbol{N}_{A,B} = N_r^{A,B}\boldsymbol{e}_r \otimes \boldsymbol{e}_r + N_\varphi^{A,B} \, \boldsymbol{e}_\varphi \otimes \boldsymbol{e}_\varphi, \quad \boldsymbol{M}_{A,B} \equiv \boldsymbol{0}, \quad \boldsymbol{n} = \sigma\boldsymbol{e}_\varphi, \quad \boldsymbol{m} = \boldsymbol{0}, \quad W_C = \sigma\frac{B}{b}, \\
&N_r^{A,B} = 2C_1^{A,B}u', \quad N_\varphi^{A,B} = 2C_1^{A,B}\frac{u}{r}.
\end{aligned}
\tag{28}
$$

Solving the equilibrium equations we obtain [1]

$$
u_{A,B}(r) = u_0^{A,B}r + \frac{u_1^{A,B}}{r},
\tag{29}
$$

where $u_0^{A,B}$ and $u_1^{A,B}$ are integration constants.

Using kinematic boundary conditions and kinematic continuity conditions

$$
u_A(a) = u^*, \quad u_A(b) = u_B(b), \quad \text{and} \quad u_B(r) \to 0 \quad \text{for} \quad r \to \infty,
\tag{30}
$$

we obtain that $u_0^B = 0$, $u_1^B = u_1^A + b^2 u_0^A$, and $u_0^A = \dfrac{u^*}{a} - \dfrac{u_1^A}{a^2}$. The integration constant u_1^A can be found from the reduced third equation (22):

$$\llbracket N\nu \rrbracket \equiv \left[N_r^A(b) - N_r^B(b) \right] e_r = \frac{\sigma}{b} e_r,$$

while the a priory unknown radius b of the phase interface circle C from the first of equations (20) or (22):

$$C_1^A \left[u_A'^2(b) + \frac{u_A^2(b)}{b^2} \right] - C_1^B \left[u_B'^2(b) + \frac{u_B^2(b)}{b^2} \right] + \Delta_A - \frac{1}{2} \left[N_r^A(b) + N_r^B(b) \right] \left[u_A'(b) - u_B'(b) \right] = \frac{\sigma B}{b^2}.$$

(31)

The two-phase solution exists only if $u^* > u_0^*$, where $u_0^* = a\,\dfrac{\bar{\sigma} c + 2\sqrt{\bar{\sigma} c^2 - \bar{\sigma} - \Delta + \bar{\sigma}^2 + \Delta c^2}}{2(c^2 - 1)}$, $c = \dfrac{C_1^B}{C_1^A} > 0$, and $\bar{\sigma} = \dfrac{\sigma}{C_1^A a}$. The solution indicates that within $0 < u^* < u_0^*$ there is only one material phase "B" in the plate. When the assumed boundary translation reaches the critical value $u^* = u_0^*$ the second more "soft" material phase "A" is created with a smaller modulus of elasticity than that of the phase "B". Finally, when $u^* > u_0^*$ the plate consists of two regions with two different material phases separated by the circular interface C of radius b. The value of b depends upon the ratio c between the material constants C_1^B and C_1^A, as well as upon $\bar{\sigma}$ and Δ (see Fig. 3).
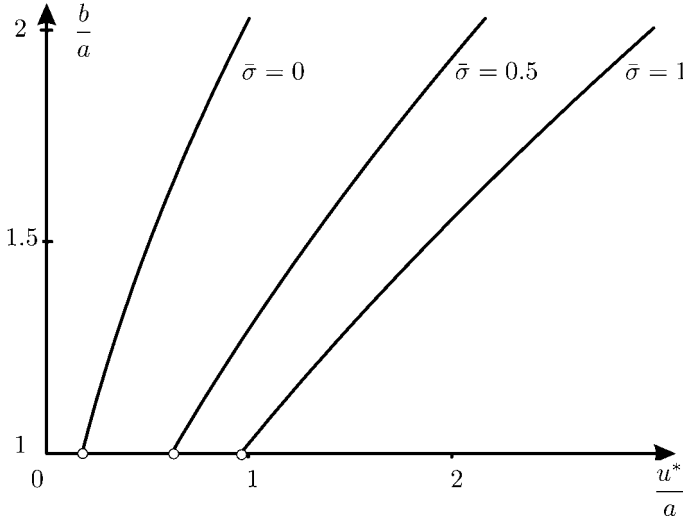

Fig. 3 Phase diagram for two-phase plate.

Note that in this problem the line tension affects position of the phase interface C if the value of $\bar{\sigma}$ is big enough. If $\bar{\sigma} \ll 1$ then in the limit $\bar{\sigma} \to 0$ we obtain the results given in [1] . In the theory of phase transitions of 3D elastic bodies [10] the surface tension essentially affects the new phase nucleation if the curvature of nucleation surface is big enough. In the example considered here the nucleation curve of the new phase is a ring which curvature is not so big to affect the phase transition for small values of the line tension.

After determining the integration constants the total energy I is a function of parameters $x \equiv b/a$ and $\bar{u} \equiv u^*/a$ and is given by the relation

$$
\begin{aligned}
\frac{1}{2\pi a^2 C_1^A} I(x, \bar{u}) = \quad & \frac{1}{c x^2 + x^2 - c + 1} \left\{ 2\bar{u}^2 \left(x^2 + c x^2 + c - 1 \right) + 2\bar{u}\bar{\sigma} x \right. \\
& + \frac{1}{4} \left[2\Delta\,(c+1)\,x^4 + 4\bar{\sigma}\,(c+1)\,x^3 - \left(4\Delta c + \bar{\sigma}^2 \right) x^2 \right. \\
& \left. \left. + 4\bar{\sigma}\,(1-c)\,x + 2\Delta c - 2\Delta + \bar{\sigma}^2 \right] \right\}.
\end{aligned}
$$

(32)

By differentiation it may be shown that Eq. (31) is equivalent to the equation $\dfrac{\partial I}{\partial x} = 0$. It is easy to show that when $u^* > u_0^*$ there exists only one solution for the phase interface circle of radius b. Dependence of the total energy (32) on b is given in Fig. 4, where only one minimum exists if $u^* > u_0^*$.
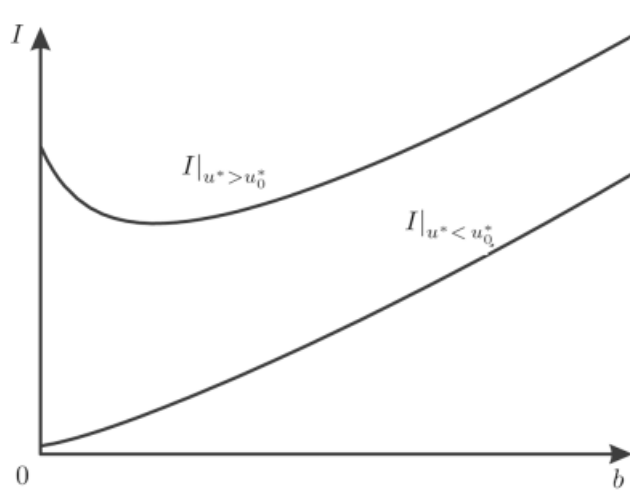
Fig. 4 Dependence of the total energy on the interface radius b for different values of u^*.
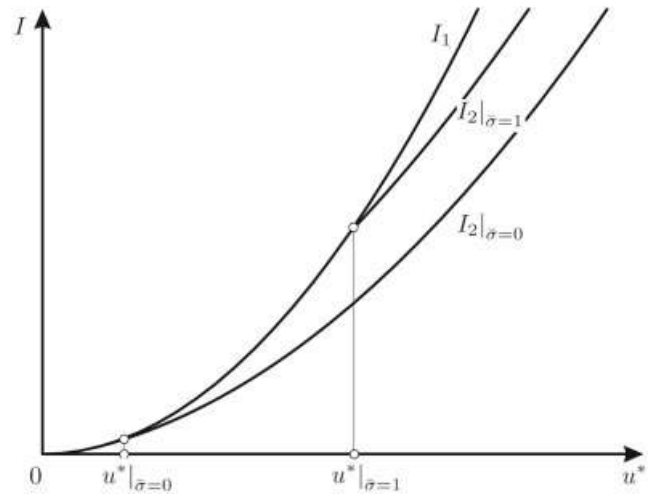
Fig. 5 Total energies for two-phase solution I_2 and for one-phase solution I_1.

The solution corresponding to the two-phase equilibrium state is energetically preferable. Let us calculate the value of the functional I on the two-phase solution as well as on the corresponding one-phase solution for different values of $\bar{\sigma}$. Then the total potential energy I_2 corresponding to the two-phase equilibrium state is always lower than I_1 corresponding to the one-phase state, see Fig. 5.

6   Conclusions

The non-linear quasi-static boundary-value problem of PTs in shells proposed in [1] has been extended by taking into account the elastic strain energy density of the interface as well as the resultant forces and couples acting along the curvilinear interface itself. From the variational principle of total potential energy we have derived the extended static natural continuity conditions to be satisfied at the interface. The conditions allow one to establish position of the interface curve in the thermodynamic equilibrium state of PT.

We have applied the general dynamically and kinematically exact shell model. Therefore, all simplified versions of shell theory with PT can be derived by an appropriate specialization of our results.

The variational principle (7) and the static natural continuity conditions (20) and (22) may be useful in determining the equilibrium position of a movable singular curve in the shell describing other types of singular phenomena. For example, by analogy to the theory of dislocations in 3D bodies [34] the approach developed here may be applied to determination of equilibrium of thin films with dislocations and/or of thin-walled structures with singular curvilinear defects of any nature.

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