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Semi-analytical analysis of thermally induced damage in thin ceramic coatings

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Abstract

An efficient procedure to analyze damage evolution in brittle coatings under influence of thermal loads is suggested. The approach is based on a general computational scheme to determine damage evolution parameters, which incorporates an analytical solution of the appropriate interim boundary-value thermoelasticity problem. For thin inhomogeneous coatings, the simplification in the analysis is achieved by application of the mathematical model with generalized boundary conditions of thermomechanical conjugation of the substrate with environment via the coating. Efficiency of the suggested approach is illustrated by an example of damage evolution in the alumina coating on the titanium-alloy and tungsten substrates under uniform heating.

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1. Introduction

The process of deposition of ceramic coatings onto (usually metallic) substrates results in formation of specific microstructures in such brittle coatings. Characteristic features of these coatings include manufacture-induced porosity and microcracks, and anisotropy in thermomechanical properties. These factors together with a significant mismatch in coefficients of thermal expansion of coatings and substrates could

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result in initiation and evolution of damage and crack generation even under purely thermal loading, in the absence of mechanical loads.

An adequate analysis of thermally induced damage evolution thus should include an additional variable, characterizing the damage state. This can be implemented in terms of Continuum Damage Mechanics (CDM). A CDM model for a damage evolution in brittle media was suggested by Najar (1987) based on thermodynamic considerations. This approach was modified in (Silberschmidt and Najar, 1998; Silberschmidt, 2003) where a computational scheme for estimation of damage evolution in bulk ceramics with different types of random microstructure is suggested. Application of this approach to a general case of thermally loaded brittle coatings presupposes numerical modeling, and respective algorithms are discussed in (Silberschmidt, 2002; Zhao and Silberschmidt, 2005). Such a cumbersome procedure to estimate parameters of the damage evolution process as well as stress, strain and temperature fields can be simplified (and enhanced) by incorporation of an analytical solution of the appropriate interim boundary-value problem of thermoelasticity into the scheme, thus resulting in an analytico-numerical approach (Shevchuk and Silberschmidt, 2003).

To obtain such type of the analytical solution for thermoelasticity problems in a case of thin inhomogeneous coatings, various approaches can be used that employ the consideration of smallness for coating thickness (Lyubimov et al., 1992; Tret'yachenko and Barilo, 1993; Suhir, 1988; Elperin and Rudin, 1998). One of the most effective schemes is based on representing the influence of thin-walled elements of structures by means of special boundary conditions (Podstrigach and Shevchuk, 1967; Pelekh and Fleishman, 1988; Shevchuk, 1997, 2000, 2002a). This approach allows reduction of the solution of a boundary-value problem for a non-homogeneous body to the problem of a homogeneous body, but with a generalized boundary, on which parameters of the homogeneous body must satisfy some complicated boundary conditions. These conditions provide an approximate relation between components of a stress tensor and a displacement vector at the body–coating interface with prescribed surface loading at the coating–environment boundary, also accounting for thermal strains in coating. Such boundary conditions describe the effect of thin coatings, simulated as shells with respective geometrical and physical properties, on the thermomechanical state of the body–coating system.

These constraints for mechanical parameters together with generalized boundary conditions (GBCs) for heat transfer (Shevchuk, 1996, 2002b) allow us to formulate and solve non-classical boundary-value problems of thermoelasticity, and to determine the stress–strain state of bodies with thin coatings under transient thermal loads.

The suggested approach, based on the use of the GBCs, was validated by comparing the approximate and exact solutions of several test problems including (a) heat conduction in a plate with a three-layer coating (Shevchuk, 2002b), (b) the test Lamé problem for mechanical loading of a solid cylinder with a three-layer coating (Shevchuk, 2000), and (c) a thermal stress state of a solid cylinder with a three-layer coating under uniform heating (Shevchuk, 2002a). This comparison has shown a fair agreement for all the analyzed cases.

The GBCs can be derived by means of different techniques. Depending on the type of boundary conditions, the following methods can be used:

- (i) the operator method, avoiding any preliminary hypotheses for the transverse distribution of the sought functions in coatings (Podstrigach and Shvets, 1978);
- (ii) the approach, using a priori assumptions for the transverse distribution of the sought functions in coatings (Podstrigach et al., 1975);
- (iii) the discrete approach based on appropriate approximations for normal derivatives by expansions (Pelekh and Fleishman, 1988).

In this study, the original model is modified to take into consideration additional features: anisotropy of ceramic coatings, inhomogeneity of the initial porosity, temperature dependence of thermomechanical

parameters of the coating and substrate as well as the dependence of the coating's elastic moduli on the damage level.

The derivation of GBCs for mechanical conjugation of the body with its environment via a thin transversely isotropic coating is based on the application of the theory of anisotropic shells (Ambartsumyan, 1974) with an account for a normal transversal strain component (Vasilenko, 1999).

Efficiency of the suggested approach (briefly outlined by Shevchuk and Silberschmidt, 2003) is illustrated in this paper by analysis of damage evolution in alumina coating on a titanium-alloy and tungsten substrates under uniform heating.

2. General computational scheme

The damage parameter, introduced into the continuum-mechanical model, characterizes the macroscopic development of failure in ceramic coatings linked to the evolution of defects at the microscopic level. The current value of the damage parameter D is determined by the local strain level and the initial damage D_0 according to the following relation for the anisotropic case:

$$D = D_0 \exp \left(\frac{E_i \langle \varepsilon_i^* \rangle^2}{2W} \right) \quad (1)$$

with the summation over all the non-negative principal elastic strains ε_i^* . Here angle brackets are Macaulay brackets, i.e. $\langle x \rangle = \begin{cases} x & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{cases}$; W is the specific energy linked with the damage evolution; E_i are Young's moduli of the undamaged transversely isotropic material. This equation generalizes damage evolution law, initially introduced for the isotropic case (Najar and Silberschmidt, 1998; Silberschmidt, 2002). The general variant of this CDM model fully describes deformational behavior and damage accumulation in brittle materials for loading and unloading/reloading conditions (see Najar (1987) and Najar and Silberschmidt (1998) for details). In this paper we deal with monotonous loading due uniform loading hence excluding strain-history effects from consideration.

An attainment of the threshold value of damage D_m due to the increase in the external load/deformation corresponds to the local failure event, i.e. a transfer from the disperse accumulation of damage to failure localization and initiation of microscopic cracking. For purely thermal loading of the substrate-coating system, linked to the increase in temperature T , the main cause of damage is the mismatch in coefficients of thermal expansions of its components.

The influence of damage on the material's behavior is introduced into the model in terms of the linear decrease of Young's moduli with the growth of damage $E_i \rightarrow E_i(1 - D)$ that is based on one of the main principles of CDM. With $D_m < 1$, a transition from the disperse damage accumulation to macroscopic failure is characterized by non-vanishing residual stiffness. Also, we take into account the temperature dependence of thermomechanical and physical parameters.

A fully analytical way to estimate the critical level of temperature changes linked to initiation of the local failure in the coating is not possible due to coupling of deformational and damage processes, and the problem is solved as an iterative sequence of steps, implemented until attainment of the damage threshold D_m . Thus, under uniform heating the following iterative procedure to determine the change of damage parameter is used:

$$D(T + \delta T) = D_0 \exp \left(\frac{E_i \langle \varepsilon_i^*(T, B_{jl}(D(T))) \rangle^2}{2W(T)} \right), \quad (2)$$

where B_{jl} are elastic coefficients for transversely isotropic body.

The general flow diagram of the computational scheme used to study damage evolution in the coating is shown in **Fig. 1**. It starts with the input of initial state. At each step of heating linked to the temperature increment δT , calculations of the stress and the strain fields and corresponding damage distribution (according to the Eq. (2)) are performed. This scheme includes a sequence of interim thermoelasticity boundary-value problems for a medium with damage. It can be implemented using the modified finite-element procedures with an account for damage evolution. Such implementation is rather cumbersome and should be based on the models accounting for the damage parameter either in a parametric form or with use of special finite elements with an additional degree of freedom (see models and respective discussions in (Silberschmidt, 2002; Zhao and Silberschmidt, 2005)). To overcome this complicacy and to obtain an effective solution algorithm, this paper utilizes a new, alternative approach based on the substitution of the finite-element solution with an analytical solution of the interim thermoelasticity problem for the body–coating system at each iteration step of a general computational iterative procedure. It should be noted that the analytical part of this semi-analytical computational procedure will consist of two consecutive stages: (1) solution of the non-classical interim thermoelasticity boundary-value problem for a body with GBCs; (2) determination of stress and strain fields in a coating by means of relations that are referred to as the

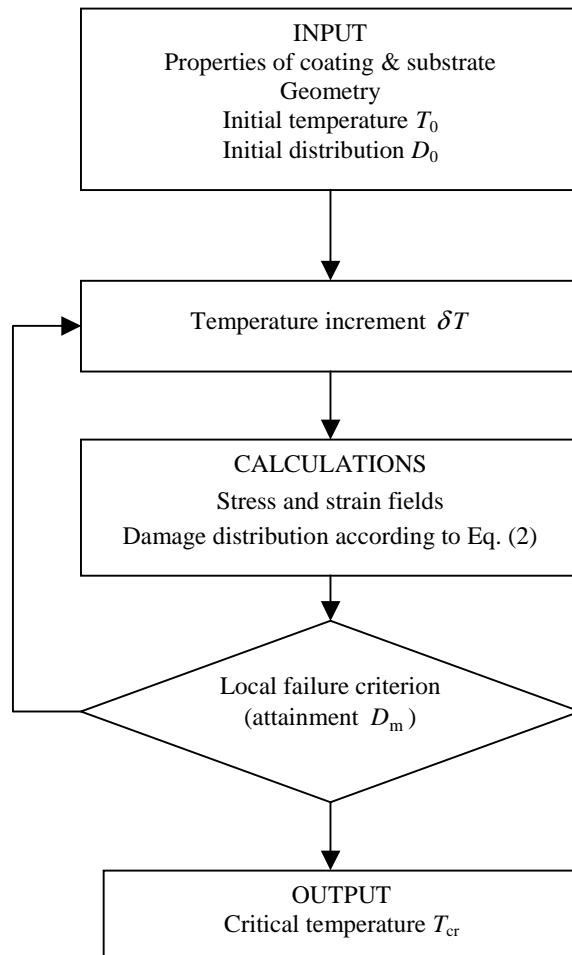


Fig. 1. Flow diagram of the general computational scheme.

restoration relations below (Sections 3 and 4). The details of this analytical part will be discussed in respective sections below.

3. Generalized boundary conditions and restoration relations

The object under study is a body with a thin ceramic coating of thickness h . Here the coating is considered as a thin shell referred to a mixed coordinate system $(\alpha_1, \alpha_2, \gamma)$, the axes of which coincide with the lines of principal curvatures of the body–coating interface and its normal (Fig. 2).

The ceramic coating is transversely isotropic with respect to its deposition direction, which coincides with the axis γ in Fig. 2. Deposition processes are usually linked with the non-vanishing porosity levels in brittle coatings. Hence, the Young moduli are considered as linearly dependent on the level of porosity; and the properties of the coating are also temperature-dependent.

We assume that the vector of tractions at the coating–environment boundary is prescribed:

$$\sigma_3^c = \sigma_3^e \quad \text{at } \gamma = h, \quad (3)$$

and the following interfacial conditions of ideal mechanical bonding between the coating and body hold

$$U_c = U_b, \quad \sigma_3^c = \sigma_3^b \quad \text{at } \gamma = 0. \quad (4)$$

Here indices c, b, and e refer to the coating, the body, and the environment, respectively; σ_3 is the stress vector, which acts on the surface $\gamma = \text{const}$, $\sigma_3^c = \sigma_{13}^c \mathbf{e}_1 + \sigma_{23}^c \mathbf{e}_2 + \sigma_{33}^c \mathbf{e}_3$; $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ are unit vectors of the coordinate trihedron linked to the base surface S_0 of the shell; $U_c = U_1^c \mathbf{e}_1 + U_2^c \mathbf{e}_2 + U_3^c \mathbf{e}_3$ is the displacement vector of points of the coating; $U_b = u_b \mathbf{e}_1 + v_b \mathbf{e}_2 + w_b \mathbf{e}_3$ is the displacement vector of points of the body on the boundary of contact with the coating.

We assume that the distribution of temperature $T(\alpha_1, \alpha_2, \gamma)$ in the coating is prescribed.

The derivation of GBCs of the mechanical conjugation of the body with its environment via a thin coating is implemented on the basis of the theory of anisotropic shells (Ambartsumyan, 1974; Grigorenko and Vasilenko, 1981; Vasilenko, 1999).

To derive these conditions, we use the Kirchhoff–Love hypothesis; however, due to the difference between Young's moduli of a transversal isotropic coating, we shall take into account the normal strain ε_3 as an additional degree of freedom (Vasilenko, 1999; Burak et al., 1978). Then geometrical relations have the form

$$\begin{aligned} U_1^c(\alpha_1, \alpha_2, \gamma) &= (1 + k_1 \gamma) u_c(\alpha_1, \alpha_2) - \frac{\gamma}{A_1} \frac{\partial w_c(\alpha_1, \alpha_2)}{\partial \alpha_1}, \\ U_2^c(\alpha_1, \alpha_2, \gamma) &= (1 + k_2 \gamma) v_c(\alpha_1, \alpha_2) - \frac{\gamma}{A_2} \frac{\partial w_c(\alpha_1, \alpha_2)}{\partial \alpha_2}, \\ U_3^c(\alpha_1, \alpha_2, \gamma) &= w_c(\alpha_1, \alpha_2) + \varepsilon_3(\alpha_1, \alpha_2) \gamma, \end{aligned} \quad (5)$$

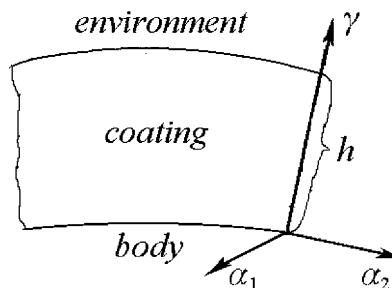


Fig. 2. Scheme of the studied object.

and appropriate relations for strains in case of a thin shell are

$$e_{11}^c = \varepsilon_1 + \kappa_1\gamma + k_1\gamma(\varepsilon_3 - \varepsilon_1), \quad e_{22}^c = \varepsilon_2 + \kappa_2\gamma + k_2\gamma(\varepsilon_3 - \varepsilon_2), \quad e_{33}^c = \varepsilon_3, \quad e_{12}^c = \varepsilon_{12} + \kappa_{12}\gamma, \quad (6)$$

where A_1 and A_2 are the Lamé parameters. Principal curvatures k_1 and k_2 , displacements u_c, v_c and w_c , and components of strains $\varepsilon_1, \varepsilon_2, \varepsilon_{12}, \kappa_1, \kappa_2$ and κ_{12} are related to the base surface S_0 .

Equilibrium equations for such shells (in the absence of body forces), given in [Vasilenko \(1999\)](#), can be written in the following form:

$$\mathbf{C}\xi + \mathbf{C}_3\xi_3 = \mathbf{B}, \quad (7)$$

where ξ and ξ_3 are the column vectors of forces and moments, which arise in the coating:

$$\xi = [N_1, N_2, N_{12}, N_{21}, Q_1, Q_2, M_1, M_2, M_{12}, M_{21}]^T, \quad \xi_3 = [N_3, M_{13}, M_{23}]^T,$$

$$\mathbf{B} = [q_1, q_2, q_3, m_1, m_2, m_3]^T,$$

$$q_j = \sigma_{j3}^c(1 + k_1h)(1 + k_2h) - \sigma_{j3}^b, \quad m_j = h\sigma_{j3}^c(1 + k_1h)(1 + k_2h), \quad j = 1, 2, 3.$$

Here \mathbf{C} and \mathbf{C}_3 are the matrices of differential operators:

$$\mathbf{C} = \frac{1}{A_1 A_2} \begin{bmatrix} -\partial_1(A_2()) & A_{2,1} & -A_{1,2} & -\partial_2(A_1()) & -k_1 A_1 A_2 & 0 & 0 & 0 & 0 & 0 \\ A_{1,2} & -\partial_2(A_1()) & -\partial_1(A_2()) & -A_{2,1} & 0 & -k_2 A_1 A_2 & 0 & 0 & 0 & 0 \\ k_1 A_1 A_2 & k_2 A_1 A_2 & 0 & 0 & -\partial_1(A_2()) & -\partial_2(A_1()) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & A_1 A_2 & 0 & -\partial_1(A_2()) & A_{2,1} & -A_{1,2} & -\partial_2(A_1()) \\ 0 & 0 & 0 & 0 & 0 & A_1 A_2 & A_{1,2} & -\partial_2(A_1()) & -\partial_1(A_2()) & -A_{2,1} \\ 0 & 0 & 0 & 0 & 0 & 0 & k_1 A_1 A_2 & k_2 A_1 A_2 & 0 & 0 \end{bmatrix},$$

$$\mathbf{C}_3 = \frac{1}{A_1 A_2} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ A_1 A_2 & -\partial_1(A_2()) & -\partial_2(A_1()) \end{bmatrix},$$

$$\begin{Bmatrix} N_i, N_{ij}, Q_i \\ M_i, M_{ij}, M_{i3} \end{Bmatrix} = \int_0^h \begin{Bmatrix} \sigma_{ii}^c, \sigma_{ij}^c, \sigma_{i3}^c \end{Bmatrix} (1 + k_j\gamma) \begin{Bmatrix} 1 \\ \gamma \end{Bmatrix} d\gamma, \quad i = 1, 2; \quad j = 3 - i,$$

$$N_3 = \int_0^h \sigma_{33}^c(1 + k_1\gamma)(1 + k_2\gamma) d\gamma,$$

a comma in a subscript followed by a subscript index denotes a partial derivative with respect to the corresponding coordinate α_l , e.g., $A_{j,l} = \partial A_j / \partial \alpha_l$; $\partial_j = \partial / \partial \alpha_j$, $j, l = 1, 2$; the empty parentheses () denote the location of an operand in respective expressions; symbol T is a sign of transposition.

Constitutive equations suggested by [Vasilenko \(1999\)](#) are modified here, and they take the form with an account for relations (6)

$$\boldsymbol{\Theta} = \mathbf{K}\boldsymbol{\varepsilon} + \mathbf{K}_3\varepsilon_3 - \boldsymbol{\Theta}_T, \quad (8)$$

where

$$\boldsymbol{\Theta} = [N_1, N_2, N_3, S, M_1, M_2, H]^T, \quad \boldsymbol{\Theta}_T = [N_{1T}, N_{2T}, N_{3T}, 0, M_T, M_T, 0]^T, \quad \boldsymbol{\varepsilon} = [\varepsilon_1, \varepsilon_2, \varepsilon_{12}, \kappa_1, \kappa_2, \kappa_{12}]^T,$$

$$\begin{Bmatrix} N_{1T}, M_T \\ N_{3T} \end{Bmatrix} = \int_0^h \begin{Bmatrix} (B_{11} + B_{12})\Phi_1 + B_{13}\Phi_3 \\ 2B_{13}\Phi_1 + B_{33}\Phi_3 \end{Bmatrix} \begin{Bmatrix} 1, \gamma \\ 1 \end{Bmatrix} d\gamma, \quad \Phi_j(T) = \int_{T_0}^T \beta_j(T') dT', \quad j = 1, 3, \quad (9)$$

$$\mathbf{K} = \begin{bmatrix} G_{11}^{(0)} & G_{12}^{(0)} & 0 & G_{11}^{(1)} & G_{12}^{(1)} & 0 \\ G_{12}^{(0)} & G_{11}^{(0)} & 0 & G_{12}^{(1)} & G_{11}^{(1)} & 0 \\ G_{13}^{(0)} & G_{13}^{(0)} & 0 & G_{13}^{(1)} & G_{13}^{(1)} & 0 \\ 0 & 0 & G_{66}^{(0)} & 0 & 0 & 2G_{66}^{(1)} \\ G_{11}^{(1)} & G_{12}^{(1)} & 0 & G_{11}^{(2)} & G_{12}^{(2)} & 0 \\ G_{12}^{(1)} & G_{11}^{(1)} & 0 & G_{12}^{(2)} & G_{11}^{(2)} & 0 \\ 0 & 0 & G_{66}^{(1)} & 0 & 0 & 2G_{66}^{(2)} \end{bmatrix}, \quad \mathbf{K}_3 = \begin{bmatrix} G_{13}^{(0)} + k_1 G_{11}^{(1)} + k_2 G_{12}^{(1)} \\ G_{13}^{(0)} + k_1 G_{12}^{(1)} + k_2 G_{11}^{(1)} \\ G_{33}^{(0)} + (k_1 + k_2) G_{13}^{(1)} \\ 0 \\ G_{13}^{(1)} + k_1 G_{11}^{(2)} + k_2 G_{12}^{(2)} \\ G_{13}^{(1)} + k_1 G_{12}^{(2)} + k_2 G_{11}^{(2)} \\ 0 \end{bmatrix}.$$

Here

$$G_{ij}^{(m)} = \int_0^h B_{ij} \gamma^m d\gamma, \quad m = 0, 1, 2, \quad ij = 11, 12, 13, 33, 66,$$

where

$$S = N_{12} - k_2 M_{21} = N_{21} - k_1 M_{12}, \quad H = (M_{12} + M_{21})/2.$$

In Eq. (8) \mathbf{K} is the matrix of elastic constants; $\boldsymbol{\epsilon}$ is the column vector of strain components of the base surface; $\boldsymbol{\theta}$ is the column vector of forces and moments in the coating; $\boldsymbol{\theta}_T$ is the column vector of parameters linked with temperature strains; elastic coefficients B_{ij} for transversely isotropic body are given in Appendix A; k_1 and k_2 are coefficients of thermal expansion in the plane of isotropy and along its normal, respectively; T_0 is the initial strain-free temperature distribution.

We assume a quadratic distribution for shear stresses σ_{j3}^c along the shell thickness (Grigorenko and Vasilenko, 1981; Ambartsumyan, 1974):

$$\sigma_{j3}^c = Q_j \frac{6\gamma(h - \gamma)}{h^3} + \sigma_{j3}^e \left(-\frac{2\gamma}{h} + \frac{3\gamma^2}{h^2} \right) + \sigma_{j3}^b \left(1 - \frac{4\gamma}{h} + \frac{3\gamma^2}{h^2} \right), \quad j = 1, 2. \quad (10)$$

Then, neglecting the terms of the higher orders of smallness (taking into account $k_1 h, k_2 h \ll 1$)

$$M_{j3} = \int_0^h \sigma_{j3}^c \gamma (1 + k_{3-j} \gamma) d\gamma = Q_j \frac{h}{2} + \left(\sigma_{j3}^e - \sigma_{j3}^b \right) \frac{h^2}{12}, \quad j = 1, 2. \quad (11)$$

Substituting (11) into (7), excluding transverse forces Q_1 and Q_2 from Eq. (7) and neglecting terms of the higher orders of smallness, we present these equations in the transformed form:

$$\begin{cases} \sigma_{j3}^b - F_j [N_1, N_2, S, M_1, M_2, H] = \sigma_{j3}^e, & j = 1, 2, \\ \sigma_{33}^b - F_3 [N_1, N_2, M_1, M_2, H] = \sigma_{33}^e + h A [\sigma_{13}^e, \sigma_{23}^e], \\ \frac{h}{2} \sigma_{33}^b - \frac{h^2}{12} A [\sigma_{13}^b, \sigma_{23}^b] + k_1 \left(\frac{h}{2} N_1 - M_1 \right) + k_2 \left(\frac{h}{2} N_2 - M_2 \right) - N_3 = -\frac{h}{2} \sigma_{33}^e - \frac{h^2}{12} A [\sigma_{13}^e, \sigma_{23}^e], \end{cases} \quad (12)$$

where

$$\begin{aligned} F_j [\varphi_1, \varphi_2, \varphi_3, \varphi_4, \varphi_5, \varphi_6] &= A_1^{-1} A_2^{-1} [\partial_j (A_l \varphi_j) - A_{l,j} \varphi_l + \partial_l (A_j \varphi_3) + A_{j,l} \varphi_3 + k_j (\partial_j (A_l \varphi_{3+j}) \\ &\quad - A_{l,j} \varphi_{3+l} + 2\partial_l (A_j \varphi_6)) + 2k_l A_{j,l} \varphi_6], \\ &j = 1, 2; \quad l = 3 - j, \end{aligned} \quad (13)$$

$$F_3[\varphi_1, \varphi_2, \varphi_3, \varphi_4, \varphi_5] = -k_1\varphi_1 - k_2\varphi_2 + A_1^{-1}A_2^{-1} \sum_{j=1}^2 \partial_j \left[A_j^{-1} (\partial_j(A_l\varphi_{2+j}) - A_{l,j}\varphi_{2+l} + \partial_l(A_j\varphi_5) + A_{j,l}\varphi_5) \right],$$

$$A[\varphi_1, \varphi_2] = A_1^{-1}A_2^{-1} (\partial_1(A_2\varphi_1) + \partial_2(A_1\varphi_2)).$$

Substituting expressions (8) and geometrical relations (Grigorenko and Vasilenko, 1981)

$$\boldsymbol{\varepsilon} = \boldsymbol{\Pi}[u_c, v_c, w_c]^T \quad \text{at } \gamma = 0, \quad (14)$$

$$\boldsymbol{\Pi} = \begin{bmatrix} \frac{\partial_1(\cdot)}{A_1} & \frac{A_{1,2}}{A_1 A_2} & k_1 \\ \frac{A_{2,1}}{A_1 A_2} & \frac{\partial_2(\cdot)}{A_2} & k_2 \\ \frac{A_1 \partial_2 \left(\frac{\cdot}{A_1} \right)}{A_2} & \frac{A_2 \partial_1 \left(\frac{\cdot}{A_2} \right)}{A_1} & 0 \\ \frac{\partial_1(k_1(\cdot))}{A_1} & \frac{k_2 A_{1,2}}{A_1 A_2} & -\frac{1}{A_1} \partial_1 \left(\frac{\partial_1(\cdot)}{A_1} \right) - \frac{A_{1,2}}{A_1 A_2^2} \partial_2(\cdot) \\ \frac{k_1 A_{2,1}}{A_1 A_2} & \frac{\partial_2(k_2(\cdot))}{A_2} & -\frac{1}{A_2} \partial_2 \left(\frac{\partial_2(\cdot)}{A_2} \right) - \frac{A_{2,1}}{A_1^2 A_2} \partial_1(\cdot) \\ k_1 \frac{A_1}{A_2} \partial_2 \left(\frac{\cdot}{A_1} \right) & k_2 \frac{A_2}{A_1} \partial_1 \left(\frac{\cdot}{A_2} \right) & -\frac{1}{A_1 A_2} \left(\partial_1 \partial_2(\cdot) - \frac{A_{1,2}}{A_1} \partial_1(\cdot) - \frac{A_{2,1}}{A_2} \partial_2(\cdot) \right) \end{bmatrix}$$

between components of strains of the reference body–coating interface and displacements of this surface into transformed equilibrium Eq. (12) and taking into account the continuity condition for displacements on the body–coating interface (4), we obtain the relations

$$\begin{cases} \sigma_{j3}^b + L_{j1}u_b + L_{j2}v_b + L_{j3}w_b + p_{je}\varepsilon_3 = \sigma_{j3}^e - A_j^{-1}(\partial_j N_{1T} + k_j \partial_j M_T), \quad j = 1, 2, \\ \sigma_{33}^b + L_{31}u_b + L_{32}v_b + L_{33}w_b + p_{3e}\varepsilon_3 = \sigma_{33}^e + hA[\sigma_{13}^e, \sigma_{23}^e] + (k_1 + k_2)N_{1T} - \Delta M_T, \\ -\frac{h}{2}\sigma_{33}^b + \frac{h^2}{12}A[\sigma_{13}^b, \sigma_{23}^b] + L_{41}u_b + L_{42}v_b + L_{43}w_b + p_{4e}\varepsilon_3 \\ = \frac{h}{2}\sigma_{33}^e + \frac{h^2}{12}A[\sigma_{13}^e, \sigma_{23}^e] - (k_1 + k_2)\left(\frac{h}{2}N_{1T} - M_T\right) + N_{3T}, \end{cases} \quad (15)$$

where expressions for differential operators L_{jl} ($j, l = 1, 2, 3$) are given in Appendix B,

$$L_{4j} = A_j^{-1}(\tilde{g}_j^{(1)} + G_{13}^{(0)})\partial_j + \xi_{11}^{3-j}(\tilde{g}_{3-j}^{(1)} + G_{13}^{(0)}) + A_j^{-1}(\tilde{g}_j^{(2)} + G_{13}^{(1)})k_{j,j}, \quad j = 1, 2,$$

$$L_{43} = (k_1^2 + k_2^2)\tilde{G}_{11}^{(1)} + 2k_1k_2\tilde{G}_{12}^{(1)} + (k_1 + k_2)G_{13}^{(0)} - \sum_{m=1}^2 (\tilde{g}_m^{(2)} + G_{13}^{(1)})\Pi_m,$$

$$p_{je} = -A_j^{-1}(g_j^{(1)} + G_{13}^{(0)})\partial_j - \xi_{11}^{3-j}(G_{11}^{(1)} - G_{12}^{(1)})(k_j - k_{3-j}) - A_j^{-1}(G_{11}^{(1)}k_{j,j} + G_{12}^{(1)}k_{3-j,j}),$$

$$\begin{aligned} p_{3e} = & -\frac{G_{11}^{(2)}}{A_1 A_2} \sum_{m=1}^2 \partial_m \left(\frac{(A_{3-m}k_m)_{,m} - A_{3-m,m}k_{3-m}}{A_m} \right) - \sum_{m=1}^2 A_m^{-2}(G_{11}^{(2)}k_{m,m} + G_{12}^{(2)}k_{3-m,m})\partial_m - G_{13}^{(1)}\Delta \\ & - \sum_{m=1}^2 g_m^{(2)}\Delta_m + (k_1^2 + k_2^2)G_{11}^{(1)} + 2k_1k_2G_{12}^{(1)} + (k_1 + k_2)G_{13}^{(0)}, \end{aligned}$$

$$p_{4e} = G_{33}^{(0)} + (k_1^2 + k_2^2)\tilde{G}_{11}^{(2)} + 2k_1k_2\tilde{G}_{12}^{(2)} + (k_1 + k_2)(\tilde{G}_{13}^{(1)} + G_{13}^{(1)}),$$

$$\Delta = \frac{1}{A_1 A_2} \left(\partial_1 \left(\frac{A_2}{A_1} \partial_1 \right) + \partial_2 \left(\frac{A_1}{A_2} \partial_2 \right) \right), \quad \Delta_j = \frac{1}{A_1 A_2} \partial_j \left(\frac{A_{3-j}}{A_j} \partial_j \right), \quad j = 1, 2,$$

$$\tilde{G}_{1j}^{(m)} = G_{1j}^{(m)} - \frac{h}{2} G_{1j}^{(m-1)}, \quad j = 1, 2, 3, \quad m = 1, 2,$$

$$g_j^{(m)} = k_j G_{11}^{(m)} + k_{3-j} G_{12}^{(m)}, \quad \tilde{g}_j^{(m)} = k_j \tilde{G}_{11}^{(m)} + k_{3-j} \tilde{G}_{12}^{(m)},$$

$$\Pi_j = A_j^{-1} \partial_j (A_j^{-1} \partial_j) - \xi_{12}^j \partial_{3-j}, \quad \xi_{n_1 n_2}^j = \frac{A_{j,3-j}}{A_j^{n_1} A_{3-j}^{n_2}}, \quad j = 1, 2, \quad n_1, n_2 = 0, 1, 2, \dots$$

Excluding ε_3 from these equations, we obtain

$$\left\{ \begin{array}{l} \sigma_{j3}^b + \frac{h}{2} d_j \sigma_{33}^b - \frac{h^2}{12} d_j A[\sigma_{13}^b, \sigma_{23}^b] + \tilde{L}_{j1} u_b + \tilde{L}_{j2} v_b + \tilde{L}_{j3} w_b = \sigma_{j3}^e - \frac{h}{2} d_j \sigma_{33}^e - \frac{h^2}{12} d_j A[\sigma_{13}^e, \sigma_{23}^e] \\ \quad + \left(\frac{h}{2} (k_1 + k_2) d_j - A_j^{-1} \partial_j \right) N_{1T} - d_j ((k_1 + k_2) M_T + N_{3T}) - A_j^{-1} k_j \partial_j M_T, \quad j = 1, 2, \\ (1 + \frac{h}{2} d_3) \sigma_{33}^b - \frac{h^2}{12} d_3 A[\sigma_{13}^b, \sigma_{23}^b] + \tilde{L}_{31} u_b + \tilde{L}_{32} v_b + \tilde{L}_{33} w_b \\ \quad = (1 - \frac{h}{2} d_3) \sigma_{33}^e + \left(h - \frac{h^2}{12} d_3 \right) A[\sigma_{13}^e, \sigma_{23}^e] - ((k_1 + k_2) d_3 + \Delta) M_T \\ \quad + (k_1 + k_2) (1 + \frac{h}{2} d_3) N_{1T} - d_3 N_{3T}, \end{array} \right. \quad (16)$$

where

$$d_j = \frac{p_{je}}{p_{4e}}, \quad \tilde{L}_{ji} = L_{ji} - d_j L_{4i}, \quad j, i = 1, 2, 3.$$

Since relations (16) establish the connection between components of the stress tensor and the vector of displacements at the boundary of the body with the prescribed components of surface loading that account for thermal strains in the coating, they can be interpreted as the generalized boundary conditions for mechanical variables of the body. In other words, they represent GBCs of mechanical conjugation of a body with its environment via a thin coating. These conditions enhance the ones given by Shevchuk (2002a) due to an account for the effect of the normal strain in the coating.

Thus, the solution of the interim boundary-value thermoelasticity problem is reduced to a solution of the problem for the body with the GBCs (16). After solving this problem, it is possible to use restoration relations for stress-strain factors in the coating in terms of the boundary values for components of the stress tensor and displacement vector of the body at the body-coating interface and known parameters linked with the prescribed temperature change.

The restoration relations can be obtained in the following way. It follows from Eq. (15)₃ that

$$\begin{aligned} \varepsilon_3 = \frac{1}{p_{4e}} & \left[\frac{h}{2} (\sigma_{33}^e + \sigma_{33}^b) + \frac{h^2}{12} A[\sigma_{13}^e - \sigma_{13}^b, \sigma_{23}^e - \sigma_{23}^b] - L_{41} u_b - L_{42} v_b - L_{43} w_b \right. \\ & \left. - (k_1 + k_2) \left(\frac{h}{2} N_{1T} - M_T \right) + N_{3T} \right]. \end{aligned} \quad (17)$$

Substitution of the first continuity condition given in Eq. (4) into Eq. (14) gives other strain components of the coating-body interface:

$$\boldsymbol{\varepsilon} = \mathbf{\Pi}[\mathbf{u}_b, \mathbf{v}_b, \mathbf{w}_b]^T. \quad (18)$$

Substitution of relations (17) and (18) into Eq. (6) makes it possible to determine the total strains, and, finally, to obtain appropriate relations for the principal elastic strains in the coating:

$$\varepsilon_i^* = \varepsilon_i + \kappa_i \gamma + k_i \gamma (\varepsilon_3 - \varepsilon_i) - \Phi_1(T), \quad i = 1, 2; \quad \varepsilon_3^* = \varepsilon_3 - \Phi_3(T). \quad (19)$$

The use of relations (17) and (18) in constitutive Eq. (8) allows calculation of forces and moments in the coating. For the suggested analytical procedure, the bloc “Calculations” of the general computational scheme (see Fig. 1) comprises the following steps:

- (i) determination of the stress and strain fields in a body as a solution of the interim boundary-value thermoelasticity problem with GBCs (16);
- (ii) determination of the principal elastic strains in a coating using restoration relations (19) with an account for Eqs. (17) and (18);
- (iii) calculation of the damage distribution according to Eq. (2).

4. Case of absence of bending and twisting strains

For the particular case of the stress–strain state, characterized by the absence of *bending strains and twisting of the body–coating interface* ($\kappa_1 = \kappa_2 = \kappa_{12} = 0$), we can obtain a simplified variant of the GBCs that contain *only components of the stress tensor*.

In this case, due to continuity of tangential strains across the coating–body interface

$$\varepsilon_1 = e_{11}^b, \quad \varepsilon_2 = e_{22}^b, \quad \varepsilon_{12} = 2e_{12}^b, \quad (20)$$

the forces and moments in the coating can be expressed only in terms of the boundary values of strain components for the body

$$\boldsymbol{\Theta} = \mathbf{K}[e_{11}^b, e_{22}^b, 2e_{12}^b, 0, 0, 0]^T + K_3 \varepsilon_3 - \boldsymbol{\Theta}_T. \quad (21)$$

The Duhamel–Neumann relations for the material of the body have the form

$$e_{jl} = \frac{1 + v_b}{E_b} \sigma_{jl} - \frac{v_b}{E_b} \sigma_{ll} \delta_{jl} + \Phi_b(T) \delta_{jl}, \quad (22)$$

where

$$\Phi_b(T) = \int_{T_0}^T \beta_b(T') dT', \quad (23)$$

E_b , v_b and β_b are the Young modulus, Poisson's ratio and the coefficient of linear thermal expansion of the body, respectively; δ_{jl} is the Kronecker symbol.

Substituting Eq. (21) into equilibrium Eq. (12) and taking into account relations (23), we get

$$\left\{ \begin{array}{l} \sigma_{j3}^b + p_{j1} \sigma_{11}^b + p_{j2} \sigma_{22}^b + p_{j3} \sigma_{33}^b + p_{j4} \sigma_{12}^b + p_{jT} \Phi_b(T_b) + p_{je} \varepsilon_3 \\ \quad = \sigma_{j3}^e - A_j^{-1} (\partial_j N_{1T} + k_j \partial_j M_T), \quad j = 1, 2, \\ (1 + p_{33}) \sigma_{33}^b + p_{31} \sigma_{11}^b + p_{32} \sigma_{22}^b + p_{34} \sigma_{12}^b + p_{3T} \Phi_b(T_b) + p_{3e} \varepsilon_3 \\ \quad = \sigma_{33}^e + h A [\sigma_{13}^e, \sigma_{23}^e] + (k_1 + k_2) N_{1T} - \Delta M_T, \\ p_{41} \sigma_{11}^b + p_{42} \sigma_{22}^b + p_{43} \sigma_{33}^b + \frac{h^2}{12} A [\sigma_{13}^b, \sigma_{23}^b] + p_{4T} \Phi_b(T_b) + p_{4e} \varepsilon_3 \\ \quad = \frac{h}{2} \sigma_{33}^e + \frac{h^2}{12} A [\sigma_{13}^e, \sigma_{23}^e] - (k_1 + k_2) \left(\frac{h}{2} N_{1T} - M_T \right) + N_{3T}, \end{array} \right. \quad (24)$$

where expressions for differential operators p_{jl} ($j = 1, 2, 3$; $l = 1, 2, 3, 4$) are given in Appendix C, T_b is the boundary value of temperature at the body–coating interface,

$$p_{jT} = -A_j^{-1} (G_{11}^{(0)} + G_{12}^{(0)}) \partial_j, \quad j = 1, 2,$$

$$\begin{aligned}
p_{3T} &= (k_1 + k_2)(G_{11}^{(0)} + G_{12}^{(0)}) - (G_{11}^{(1)} + G_{12}^{(1)})\Delta, \\
p_{4j} &= E_b^{-1}(G_{13}^{(0)}(1 - v_b) + \tilde{g}_j^{(1)} - v_b \tilde{g}_{3-j}^{(1)}) \quad j = 1, 2, \\
p_{43} &= -h/2 - v_b E_b^{-1}(2G_{13}^{(0)} + (k_1 + k_2)(\tilde{G}_{11}^{(1)} + \tilde{G}_{12}^{(1)})), \\
p_{4T} &= 2G_{13}^{(0)} + (k_1 + k_2)(\tilde{G}_{11}^{(1)} + \tilde{G}_{12}^{(1)}).
\end{aligned}$$

Excluding ε_3 from these equations, we obtain finally

$$\left\{
\begin{aligned}
&\sigma_{j3}^b + \tilde{p}_{j1}\sigma_{11}^b + \tilde{p}_{j2}\sigma_{22}^b + \tilde{p}_{j3}\sigma_{33}^b + p_{j4}\sigma_{12}^b + \tilde{p}_{jT}\Phi_b(T_b) - p_{j5}\Lambda[\sigma_{13}^b, \sigma_{23}^b] \\
&= \sigma_{j3}^e - p_{j6}\sigma_{33}^e - p_{j5}\Lambda[\sigma_{13}^e, \sigma_{23}^e] + p_{j7}N_{1T} - p_{j8}N_{3T} - p_{j9}M_T, \quad j = 1, 2, \\
&(1 + \tilde{p}_{33})\sigma_{33}^b + \tilde{p}_{31}\sigma_{11}^b + \tilde{p}_{32}\sigma_{22}^b + p_{34}\sigma_{12}^b + \tilde{p}_{3T}\Phi_b(T_b) - p_{35}\Lambda[\sigma_{13}^b, \sigma_{23}^b] \\
&= (1 - p_{36})\sigma_{33}^e + (h - p_{35})\Lambda[\sigma_{13}^e, \sigma_{23}^e] + p_{37}N_{1T} - p_{38}N_{3T} - p_{39}M_T,
\end{aligned}
\right. \quad (25)$$

where

$$\begin{aligned}
p_{m5} &= \frac{h^2}{12}d_m, \quad p_{m6} = \frac{h}{2}d_m, \quad p_{m8} = d_m, \quad m = 1, 2, 3; \\
p_{m7} &= \frac{h}{2}(k_1 + k_2)d_m - A_m^{-1}\hat{\sigma}_m, \quad m = 1, 2; \quad p_{37} = (k_1 + k_2)\left(1 + \frac{h}{2}d_3\right), \\
p_{m9} &= (k_1 + k_2)d_m + A_m^{-1}k_m\hat{\sigma}_m, \quad m = 1, 2; \quad p_{39} = (k_1 + k_2)d_3 + \Delta, \\
\tilde{p}_{mn} &= p_{mn} - p_{4n}d_m, \quad m = 1, 2, 3; \quad n = 1, 2, 3, T.
\end{aligned}$$

In this case it is possible to formulate restoration relations for stress–strain factors in the coating in terms of the boundary values only of the stress tensor components for the body at the body–coating interface and known parameters linked with the prescribed temperature change.

From Eq. (24)₃ follows

$$\begin{aligned}
\varepsilon_3 &= \frac{1}{p_{4e}} \left[\frac{h}{2}\sigma_{33}^e + \frac{h^2}{12}\Lambda[\sigma_{13}^e - \sigma_{13}^b, \sigma_{23}^e - \sigma_{23}^b] - p_{41}\sigma_{11}^b - p_{42}\sigma_{22}^b - p_{43}\sigma_{33}^b - p_{4T}\Phi_b(T) \right. \\
&\quad \left. - (k_1 + k_2)\left(\frac{h}{2}N_{1T} - M_T\right) + N_{3T} \right]. \quad (26)
\end{aligned}$$

Substitution of Eq. (22) into Eq. (20) gives other components of strains:

$$\begin{aligned}
\varepsilon_1 &= \frac{1}{E_b}\sigma_{11}^b - \frac{v_b}{E_b}(\sigma_{22}^b + \sigma_{33}^b) + \Phi_b(T), \\
\varepsilon_2 &= \frac{1}{E_b}\sigma_{22}^b - \frac{v_b}{E_b}(\sigma_{11}^b + \sigma_{33}^b) + \Phi_b(T), \\
\varepsilon_{12} &= \frac{2(1 + v_b)}{E_b}\sigma_{12}^b.
\end{aligned} \quad (27)$$

Finally, the principal elastic strains in the coating are determined by relations

$$\varepsilon_i^* = \varepsilon_i + k_i\gamma(\varepsilon_3 - \varepsilon_i) - \Phi_i(T), \quad i = 1, 2; \quad \varepsilon_3^* = \varepsilon_3 - \Phi_3(T). \quad (28)$$

Respectively, the stress factors in the coating can be determined from Eq. (8) using relations (26) and (27) and taking into account $\kappa_1 = \kappa_2 = \kappa_{12} = 0$.

The general form of the analytical procedure, discussed in Section 3, remains, with substitution of Eqs. (16)–(19) with Eqs. (25)–(28), respectively.

5. Problem of a coated cylinder

As an example, we consider the problem for a solid cylinder of radius R with a perfectly bonded ceramic coating under conditions of uniform heating. The ends of the cylinder are fixed in the axial directions, and all the tractions σ_{j3}^c ($j = 1, 2, 3$) on the coating–environment boundary vanish.

Due to axial symmetry of the problem, shear stresses vanish:

$$\sigma_{12}^b = \sigma_{13}^b = \sigma_{23}^b = 0. \quad (29)$$

In this case, the first two GBCs (25) are satisfied identically, and the third one takes the following form for $r = R$:

$$(1 + \tilde{p}_{33})\sigma_{33}^b + \tilde{p}_{31}\sigma_{11}^b + \tilde{p}_{32}\sigma_{22}^b + \tilde{p}_{3T}\Phi_b(T_b) = p_{37}N_{1T} - p_{38}N_{3T} - p_{39}M_T, \quad (30)$$

where for this case

$$\begin{aligned} p_{3e} &= R^{-1}G_{13}^{(0)} + R^{-2}G_{11}^{(1)}, \quad p_{4e} = G_{33}^{(0)} + R^{-1}(\tilde{G}_{13}^{(1)} + G_{13}^{(1)}) + R^{-2}\tilde{G}_{11}^{(2)}, \\ p_{33} &= -\frac{v_b(G_{11}^{(0)} + G_{12}^{(0)})}{RE_b}, \quad p_{43} = -\frac{h}{2} - v_bE_b^{-1}\left(2G_{13}^{(0)} + \frac{\tilde{G}_{11}^{(1)} + \tilde{G}_{12}^{(1)}}{R}\right), \\ p_{3j} &= \frac{G_{1l}^{(0)} - v_bG_{1j}^{(0)}}{RE_b}, \quad p_{4j} = \frac{1}{E_b}\left(G_{13}^{(0)}(1 - v_b) + \frac{\tilde{G}_{1l}^{(1)} - v_b\tilde{G}_{1j}^{(1)}}{R}\right) \quad j = 1, 2; \quad l = 3 - j, \\ p_{3T} &= \frac{G_{11}^{(0)} + G_{12}^{(0)}}{R}, \quad p_{4T} = 2G_{13}^{(0)} + \frac{\tilde{G}_{11}^{(1)} + \tilde{G}_{12}^{(1)}}{R}, \\ p_{37} &= \frac{1}{R}\left(1 + \frac{h}{2}d_3\right), \quad p_{38} = d_3, \quad p_{39} = \frac{d_3}{R}, \quad T_b = T. \end{aligned}$$

We write the solution of equilibrium equations for the cylinder in this case in the form (Timoshenko and Goodier, 1970)

$$\sigma_{33}^b(r) = a + \frac{b}{r^2} - \frac{E_b\Phi_b(T)}{2(1 - v_b)}, \quad \sigma_{22}^b(r) = a - \frac{b}{r^2} - \frac{E_b\Phi_b(T)}{2(1 - v_b)}, \quad (31)$$

where a and b are unknown constants. We found these constants by substituting Eq. (31) into the GBC (30) and by using condition $\sigma_{33}^b|_{r=0} \neq \infty$. Then using equality $e_{11}^b \equiv 0$ (which follows from the condition for the fixed ends) and Duhamel–Neumann relations (22), we obtain finally stresses in the cylinder in the form:

$$\begin{aligned} \sigma_{33}^b = \sigma_{22}^b &= (1 + 2v_b\tilde{p}_{31} + \tilde{p}_{32} + \tilde{p}_{33})^{-1}(p_{37}N_{1T} - p_{38}N_{3T} - p_{39}M_T - (\tilde{p}_{3T} - \tilde{p}_{31}E_b)\Phi_b(T)), \\ \sigma_{11}^b &= 2v_b\sigma_{33}^b - E_b\Phi_b(T). \end{aligned} \quad (32)$$

Substituting Eqs. (32) and (29) into restoration relations (26)–(28), we find the principal non-negative elastic strains in the coating

$$\begin{aligned}\varepsilon_3^* &= \varepsilon_3 - \Phi_3(T), \\ \varepsilon_2^* &= \varepsilon_2 + R^{-1}\gamma(\varepsilon_3 - \varepsilon_2) - \Phi_1(T),\end{aligned}\quad (33)$$

where

$$\begin{aligned}\varepsilon_3 &= -\frac{1}{p_{4e}}[(2v_b p_{41} + p_{42} + p_{43})\sigma_{33}^b + (p_{4T} - p_{41}E_b)\Phi_b(T) + 0.5hR^{-1}N_{1T} - R^{-1}M_T - N_{3T}], \\ \varepsilon_2 &= (1 + v_b)\left(\frac{1 - 2v_b}{E_b}\sigma_{33}^b + \Phi_b(T)\right).\end{aligned}\quad (34)$$

Here thermal strains $\Phi_j(T)$ ($j = 1, 3, b$) and quantities N_{1T} , N_{3T} , M_T , defined by relations (9) and (23), are known since temperature T is a prescribed parameter at uniform heating.

Thus, Eq. (33) of the closed-form solution of the interim boundary-value thermoelasticity problem provide the necessary data for the right-hand part of Eq. (2) to calculate the damage distribution at each step of uniform heating.

6. Numerical results

Analysis of damage evolution in ceramic coating on the cylindrical metallic substrate based on the solution obtained in the previous section is implemented according to the suggested semi-analytical scheme given in Section 2. A case of a long cylinder with radius 5 cm, fixed at its ends and coated with a 500 μm layer of alumina, is considered. Three types of the through-thickness distribution of the initial damage linked to the manufacture-induced porosity are analyzed: (1) uniform with the magnitude $D_0 = (D_{\min} + D_{\max})/2$, (2) linearly increasing from D_{\min} at the coating-substrate interface to D_{\max} at the external free surface (referred to as *Type 1* below), and (3) linearly decreasing from D_{\max} at the interface to D_{\min} at the surface (*Type 2*). In numerical calculations $D_{\min} = 0.02$ and $D_{\max} = 0.10$ are used, resulting in $D_0 = 0.06$. These three types of coatings are studied for two cases of the substrate's material: tungsten and Ti–6Al–4V alloy. We consider the system under purely uniform thermal loading and assume a stress- and strain-free initial state.

The properties for the coating and substrates are given in Tables 1 and 2. In the numerical part of our analysis we use cubic spline approximation for the temperature-dependent parameters from Table 1. Transversal isotropy of the alumina coating is accounted in terms of the ratio of Young's moduli E_{\parallel}/E_{\perp} , where E_{\parallel} and E_{\perp} are elastic moduli along the axial and radial directions, respectively. This ratio is varied in the interval 1–4 in calculations for Figs. 6 and 7 with the fixed value $E_{\parallel} = 150$ GPa. The influence of damage on the material's behavior is implemented by transitions (Silberschmidt, 2002; Sevostianov and Kachanov, 2001)

$$\left\{ \begin{array}{l} E_{\perp(\parallel)} \\ v_{\perp(\parallel)} \end{array} \right\} \rightarrow \left\{ \begin{array}{l} E_{\perp(\parallel)} \\ v_{\perp(\parallel)} \end{array} \right\} (1 - D).$$

Here, according to Sevostianov and Kachanov (2001) we have $v_{\perp} = v_{\parallel}E_{\perp}/E_{\parallel}$.

Table 1
Temperature-dependent material properties of coating and substrates used in numerical calculations

T (°C)	W (kJ/m ³)	Coefficients of thermal expansion $\beta_1 = \beta_3, \times 10^{-6}$ (°C ⁻¹)		
		Alumina	Tungsten	Ti–6Al–4V
100	51.2	5.02	4.4	8.64
200	50.1	5.54	4.4	9.14
300	48.8	6.06	4.4	9.47
400	47.5	6.58	4.4	9.74

Table 2
Elastic properties of coating and substrates used in numerical calculations

	Alumina	Tungsten	Ti-6Al-4V
E_{\parallel} (GPa)	150	400	114
E_{\perp} (GPa)	100	400	114
v_{\parallel}	0.24	0.28	0.33

The type of the substrate considerably affects the character of damage accumulation in ceramics (Fig. 3), though the main stages of the process are present in both cases: a relatively slow damage development at the initial stage is succeeded by a sharp increase in the damage level at the final stage. The specific position—at the interface—is chosen since calculations have shown that it is the area with the highest rate of the temperature-induced damage growth. The analysis of results demonstrates that the type of the through-thickness distribution of damage remains the same (Figs. 4 and 5) for thin coatings, treated here, in contrast to the case of thick ones (Silberschmidt, 2002). This can be explained by low variations of strains across thickness for such thin coatings. But there is a common feature of the process: non-uniform distributions of initial porosity are more dangerous with regard to the crack initiation than the uniform one.

An important parameter of purely thermal loading of coated components is the critical temperature T_{cr} of the macroscopic fracture initiation. It could be related to attainment of the critical damage level D_m in some part of the coating; overcoming this threshold means a transition from the disperse damage accumulation to failure localization in the form of a macroscopic crack. It follows from the simulations that the decrease in D_m , corresponding to the local failure initiation, results in the decline of T_{cr} for both cases of substrates and all types of coatings (Fig. 5).

It is obvious that the transition to macroscopic fracture is controlled mainly by the highest local level of the initial porosity, hence the considerable differences between the uniform distribution and two non-uniform ones. The difference between the latter two cases is rather small for thin coatings with Type 2 still being the most dangerous one as was also the case in (Silberschmidt, 2002). The suggested semi-analytical scheme reproduces the main features of thermally induced damage accumulation obtained by means of

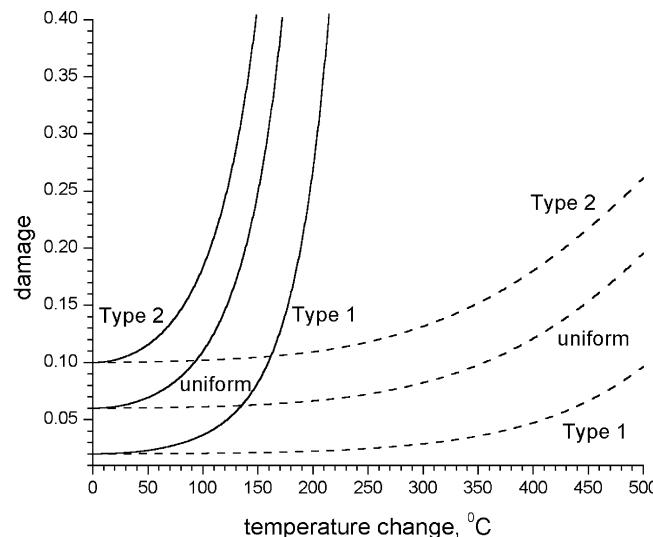


Fig. 3. Influence of temperature on damage evolution near interface for various types of initial distribution of damage for case of titanium-alloy (solid curves) and tungsten (dashed curves) substrates.

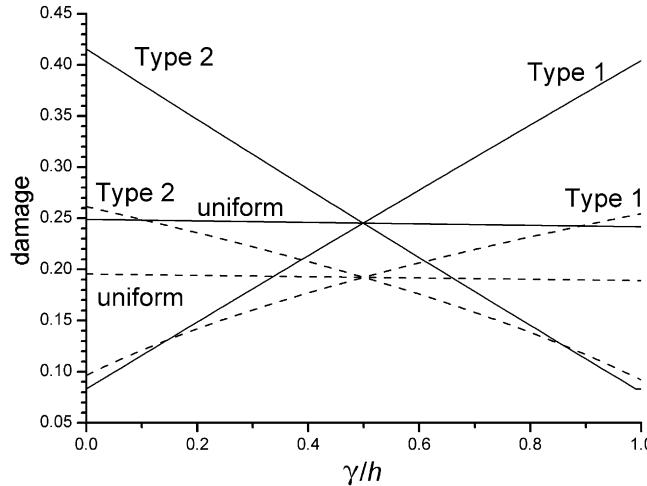


Fig. 4. Damage distributions induced by thermal changes $\delta T = 150$ °C for case of titanium-alloy substrate (solid curves) and $\delta T = 500$ °C for case of tungsten substrate (dashed curves) for various types of initial distribution of damage.

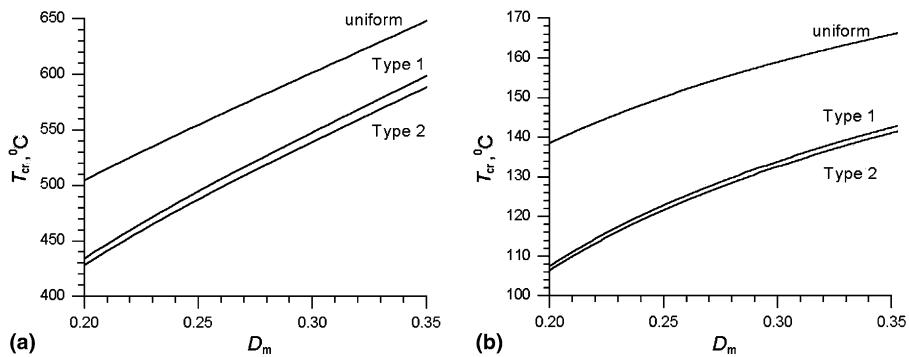


Fig. 5. Critical temperatures for varying damage threshold: (a) tungsten substrate and (b) titanium-alloy substrate.

finite elements for three studied types of alumina coatings (Silberschmidt, 2002) and provides quantitative information on both damage distribution and critical temperature that could be experimentally measured (Zhao and Silberschmidt, 2005).

The next stage of the study is to analyze the effect of manufacturing-induced anisotropy of alumina coating on damage evolution, which is essential for the case of the tungsten substrate (Figs. 6 and 7). In contrast, the influence of anisotropy for all studied cases of an alumina coating on the titanium-alloy substrate is negligibly small (deviations do not exceed 0.1%). The difference between results for two substrates is due to various types of the mismatch in coefficients of thermal expansion of the substrate and coating (see Table 1). From Eqs. (33), (34) and (32) we can obtain the following asymptotic expressions (with account for relations from Appendix A) for elastic parts of the principal strains for a very thin coating ($h/R \rightarrow 0$):

$$\varepsilon_3^* \approx \frac{E_{\parallel} v_{\perp}}{E_{\perp} (1 - v_{\parallel})} (2\Phi_1(T) - (1 + v_b)\Phi_b(T)),$$

$$\varepsilon_2^* \approx (1 + v_b)\Phi_b(T) - \Phi_1(T).$$

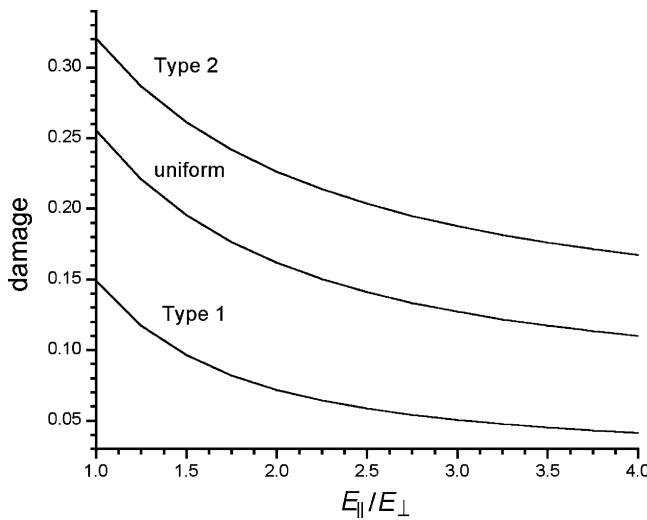


Fig. 6. Influence of ratio E_{\parallel}/E_{\perp} on level of damage near interface induced by thermal loading of $\delta T=500$ $^{\circ}\text{C}$ for various types of initial porosity (tungsten substrate).

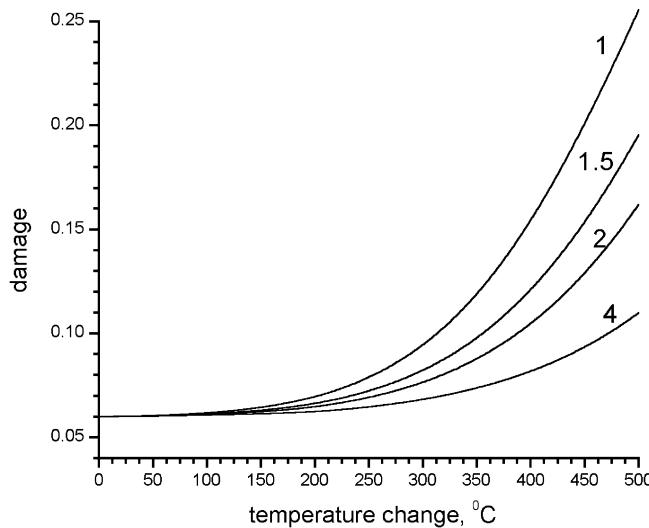


Fig. 7. Damage evolution near interface for case of uniform initial porosity for various values of Young's moduli E_{\parallel}/E_{\perp} (tungsten substrate).

Obviously, for the titanium-alloy substrate only the circumferential strain will be positive for a given type of thermal excursions, with the positive radial strain being the main factor for the tungsten substrate.

The decrease in the anisotropy accelerates damage accumulation for all types of coatings (i.e., distributions of the initial porosity) with the uniform coating being the most resistant to thermal damage from three analyzed types. Fig. 7 demonstrates damage development under conditions of the increasing temperature in the coating with a uniform distribution of the initial porosity. Here, a two-fold increase in the level of anisotropy causes halving of damage accumulation rate. As calculations show, the similar effect of ratio E_{\parallel}/E_{\perp} is observed for other two types of coatings.

7. Conclusions

In this paper, the efficient semi-analytical approach to analyze damage evolution in structural elements with ceramic coatings under influence of thermal loads has been developed. The approach employs a general computational scheme as an iterative procedure for determining damage evolution parameters, which incorporates an analytical solution of the appropriate interim boundary-value thermoelasticity problem at each iteration step. For inhomogeneous thin ceramic coatings, the simplification in the solution procedure is achieved by means of application of the mathematical model with generalized boundary conditions for thermomechanical conjugation of the substrate with environment via the coating. These conditions for ceramic coatings take into account such features as their transversal anisotropy, spatial (through-thickness) inhomogeneity of the initial porosity, temperature-dependent thermomechanical properties of the coating and substrate as well as the dependence of the coating's elastic moduli on the damage level.

The suggested analytico-numerical approach has the following advantages as compared to the use of the finite-element analysis and other direct numerical methods: (i) it notably simplifies calculations of structures with thin coatings thus ensuring essential reduction of computational efforts; (ii) it provides a possibility of important a priori qualitative and quantitative evaluation of the effects of various geometrical and thermomechanical parameters of the body–coating system on the character of the damage evolution process, while parametric studies which use universal numerical methods are exceedingly cumbersome; (iii) the efficiency of the approach based on the GBCs increases with the decrease of the coating thickness in contrast to direct methods without preliminary transformation of initial problems; (iv) it allows us to verify other computational techniques.

Based on the suggested approach, the performed numerical calculations allowed us to investigate essential features of damage evolution processes under uniform heating of the component with the alumina coating for two different substrates. It has been established that

- the type of the substrate considerably affects the character and rate of damage accumulation in ceramic coatings;
- the character of the through-thickness non-uniformity of the initial damage distribution changes insignificantly for thin coatings in contrast to the case of thick ones;
- the non-uniform distribution of initial porosity is more dangerous than uniform;
- the effect of manufacturing-induced anisotropy of the alumina coating on damage evolution is absent in the case of a titanium-alloy substrate, although it is essential for the tungsten substrate due to a different type of the mismatch in coefficients of thermal expansion between the substrates and coating.

Appendix A

Expressions for elastic coefficients B_{ij} for transversely isotropic body follow from the anisotropic ones given by [Vasilenko \(1999\)](#):

$$B_{11} = \Omega^{-1}(a_{11}a_{33} - a_{13}^2), \quad B_{12} = \Omega^{-1}(a_{13}^2 - a_{12}a_{33}), \quad B_{13} = \Omega^{-1}(a_{12} - a_{11})a_{13},$$

$$B_{33} = \Omega^{-1}(a_{11}^2 - a_{12}^2), \quad B_{66} = a_{66}^{-1}, \quad \Omega = (a_{11} - a_{12})((a_{11} + a_{12})a_{33} - 2a_{13}^2),$$

where elastic constants a_{ij} are expressed by means of engineering constants (Young's moduli, shear modulus and Poisson's ratio) as follows:

$$a_{11} = 1/E_1, \quad a_{33} = 1/E_3, \quad a_{12} = -v_{21}/E_1, \quad a_{13} = -v_{31}/E_1 = -v_{13}/E_3, \quad a_{66} = 1/G_{12}.$$

Here $E_1 = E_{\parallel}$ and $E_3 = E_{\perp}$ are Young's moduli in the plane of isotropy and in a direction normal to it, respectively; $\nu_{21} = \nu_{\parallel}$ is Poisson's ratio, characterizing transverse contraction in the plain of isotropy when tension is applied in the plane; $\nu_{13} = \nu_{\perp}$ is Poisson's ratio, characterizing transverse contraction in the plain of isotropy when tension is applied in a direction normal to the plane of isotropy; G_{12} is the shear modulus for the plane of isotropy.

Appendix B

Expressions for differential operators L_{jl} ($j, l = 1, 2, 3$) given by Shevchuk (2000) for an isotropic case are transformed for a transversely isotropic shell as follows:

$$\begin{aligned} L_{jl} = & -\frac{G_{1\rho}^{(0)}}{A_j A_l} \partial_j \partial_l - \frac{G_{66}^{(0)}}{A_{3-j} A_{3-l}} \partial_{3-j} \partial_{3-l} - \frac{G_{11}^{(0)}}{A_1 A_2} \partial_j \left(\frac{A_{3-l}}{A_j} \right) \partial_j - \frac{G_{66}^{(0)}}{A_1 A_2} \partial_{3-j} \left(\frac{A_j}{A_{3-l}} \right) \partial_{3-j} - \frac{G_{1\rho}^{(1)}}{A_j A_l} k_{l,l} \partial_j \\ & - \frac{G_{11}^{(0)} + G_{66}^{(0)}}{A_1 A_2} \left(\frac{A_{j,l}}{A_j} \partial_j - \frac{A_{l,j}}{A_l} \partial_l \right) + G_{1\rho}^{(0)} \xi_{11}^{3-j} \xi_{11}^{3-l} + G_{66}^{(0)} \xi_{11}^j \xi_{11}^l - \frac{G_{1s}^{(0)}}{A_1 A_2} \partial_j \left(\frac{A_{3-l,l}}{A_j} \right) + \frac{G_{66}^{(0)}}{A_1 A_2} \partial_{3-j} \left(\frac{A_{l,3-l}}{A_{3-j}} \right) \\ & - \frac{G_{1\rho}^{(1)}}{A_1 A_2} \partial_j \left(\frac{A_{3-l}}{A_l} k_{l,l} \right) + \frac{G_{1s}^{(1)} A_{3-j,j}}{A_l^2 A_{3-l}} k_{l,l}, \end{aligned}$$

$$\begin{aligned} L_{j3} = & \frac{G_{11}^{(1)}}{A_j^3} \partial_j^3 + \frac{G_{12}^{(1)} + 2G_{66}^{(1)}}{A_j A_{3-j}^2} \partial_j \partial_{3-j}^2 + \frac{G_{11}^{(1)}}{A_{3-j}} \partial_j \left(\frac{A_{3-j}}{A_j^3} \right) \partial_j^2 + \left(G_{11}^{(1)} \xi_{22}^j - (G_{12}^{(1)} + 2G_{66}^{(1)}) \eta_{13}^j \right) \partial_1 \partial_2 \\ & - \left(G_{11}^{(1)} + G_{12}^{(1)} + 2G_{66}^{(1)} \right) \xi_{31}^{3-j} \partial_{3-j}^2 - \left(\zeta_j - \frac{G_{12}^{(1)} - G_{11}^{(1)}}{A_j^2 A_{3-j}} \partial_j (\xi_{01}^{3-j}) \right) \partial_j \\ & - \left(\frac{G_{11}^{(1)}}{A_j} \partial_j \left(\frac{A_j}{A_{3-j}^3} \partial_{3-j} \left(\frac{A_{3-j}}{A_j} \right) \right) + \frac{G_{11}^{(1)} - G_{12}^{(1)} - 2G_{66}^{(1)}}{A_j^2 A_{3-j}} \partial_{3-j} \left(A_j \partial_j (A_{3-j}^{-1}) \right) - \frac{G_{66}^{(1)} A_{3-j,12}}{A_j A_{3-j}^3} \right) \partial_{3-j} \\ & - \left(G_{11}^{(0)} - G_{12}^{(0)} \right) (k_j - k_{3-j}) \xi_{11}^{3-j} - A_j^{-1} \left(G_{11}^{(0)} k_{j,j} + G_{12}^{(0)} k_{3-j,j} \right), \end{aligned}$$

$$\begin{aligned} L_{3j} = & -\frac{G_{11}^{(1)}}{A_j^3} \partial_j^3 - \frac{G_{12}^{(1)} + 2G_{66}^{(1)}}{A_j A_{3-j}^2} \partial_j \partial_{3-j}^2 - \frac{G_{11}^{(1)}}{A_{3-j}^2} \partial_j \left(A_j^{-3} A_{3-j}^2 \right) \partial_j^2 + \left(G_{11}^{(1)} \xi_{22}^j + (G_{12}^{(1)} + 2G_{66}^{(1)}) \eta_{13}^j \right) \partial_1 \partial_2 \\ & - G_{11}^{(1)} \xi_{31}^{3-j} \partial_{3-j}^2 + \left(\zeta_j + G_{11}^{(1)} (\xi_{14}^{3-j} \eta_{00}^{3-j} + A_1^{-1} A_2^{-1} \partial_{3-j} (\xi_{11}^j)) - G_{12}^{(1)} A_j^{-2} A_{3-j}^{-1} \partial_j (\xi_{01}^{3-j}) \right) \partial_j \\ & - \left(\frac{G_{11}^{(1)}}{A_{3-j,j}} \partial_{3-j} (\xi_{31}^{3-j} \xi_{00}^{3-j}) + (G_{11}^{(1)} - G_{12}^{(1)} - 2G_{66}^{(1)}) \xi_{23}^j \xi_{00}^{3-j} \right) \partial_{3-j} + g_{3-j}^{(0)} \xi_{11}^{3-j} \\ & + A_1^{-1} A_2^{-1} \left\{ \sum_{m=1}^2 G_{1i}^{(1)} \left[\partial_m (\xi_{12}^{3-m} A_{3-j,j}) - \partial_{3-m} \left(A_{3-m}^{-1} \partial_{3-m} \left(\frac{A_{3-j,j}}{A_{3-m}} \right) \right) \right] + G_{66}^{(1)} \partial_m \left(A_m^{-2} \partial_{3-m} \left(\frac{A_m A_{j,3-j}}{A_{3-m}} \right) \right) \right. \\ & \left. - G_{1i}^{(2)} \left[\partial_m \left(A_m^{-1} \partial_m \left(\frac{A_{3-j}}{A_m} k_{j,j} \right) \right) + \partial_m \left(\frac{A_{3-j}}{A_m^2} k_{j,j} \partial_m (\cdot) \right) - \partial_{3-m} (A_{3-m}^{-1} \xi_{01}^{3-j} k_{j,j}) \right] \right\}, \end{aligned}$$

$$\begin{aligned}
L_{33} = & \sum_{m=1}^2 \left\{ \left(G_{11}^{(2)} \Delta_m + G_{12}^{(2)} \Delta_{3-m} - g_m^{(1)} \right) \Pi_m - \left(G_{11}^{(1)} \Delta_m + G_{12}^{(1)} \Delta_{3-m} \right) k_m - \frac{G_{11}^{(1)} - G_{12}^{(1)}}{A_1 A_2} \partial_m (\xi_{01}^{3-m} (k_m - k_{3-m})) \right. \\
& + \frac{G_{11}^{(2)} - G_{12}^{(2)}}{A_1 A_2} \partial_m (\xi_{01}^{3-m} \Pi_1 - \xi_{10}^{3-m} \Pi_2) - \frac{2 G_{66}^{(2)}}{A_1 A_2} \partial_m \left(2 \xi_{21}^m X + \partial_{3-m} \left(\frac{X}{A_1 A_2} \right) \right) \left. \right\} + G_{11}^{(0)} (k_1^2 + k_2^2) \\
& + 2 G_{12}^{(0)} k_1 k_2.
\end{aligned}$$

Here,

$$\eta_{n_1 n_2}^j = \frac{A_{3-j, 3-j}}{A_j^{n_1} A_{3-j}^{n_2}}, \quad \zeta_j = A_j^{-1} [g_j^{(0)} - G_{11}^{(1)} \partial_j (A_1^{-1} A_2^{-1} \partial_j (A_j^{-1} A_{3-j})) + 2 G_{66}^{(1)} A_1^{-1} A_2^{-1} \partial_{3-j} (\xi_{01}^j)],$$

$$X = \partial_1 \partial_2 - \xi_{10}^1 \partial_1 - \xi_{10}^2 \partial_2,$$

$$j, l = 1, 2, \quad \rho = 2 - \delta_{jl}, \quad s = 1 + \delta_{jl}, \quad i = 2 - \delta_{jm}, \quad n_1, n_2 = 0, 1, 2, \dots,$$

$$\delta_{jl} = \begin{cases} 1, & j = l, \\ 0, & j \neq l \end{cases} \text{ is the Kronecker symbol.}$$

Appendix C

Expressions for differential operators p_j ($j = 1, 2, 3; l = 1, 2, 3, 4$) given by Shevchuk (2000) for an isotropic case are transformed for a transversely isotropic shell as follows:

$$\begin{aligned}
p_{jl} &= A_j^{-1} \frac{v_b G_{1s}^{(0)} - G_{1\rho}^{(0)}}{E_b} \partial_j - \xi_{11}^{3-j} \frac{1 + v_b}{E_b} (-1)^{j+l} (G_{11}^{(0)} - G_{12}^{(0)}), \\
p_{j3} &= A_j^{-1} \frac{v_b (G_{11}^{(0)} + G_{12}^{(0)})}{E_b} \partial_j, \quad p_{j4} = -\frac{2(1 + v_b)}{E_b} G_{66}^{(0)} \left(A_{3-j}^{-1} \partial_{3-j} + 2 \xi_{11}^j \right), \\
p_{3j} &= \frac{g_j^{(0)} - v_b g_{3-j}^{(0)}}{E_b} + \frac{A_1^{-1} A_2^{-1}}{E_b} \left\{ (1 + v_b) (G_{12}^{(1)} - G_{11}^{(1)}) [\partial_j (\xi_{01}^{3-j} ()) - \partial_{3-j} (\xi_{01}^j ())] \right. \\
&\quad \left. - (G_{11}^{(1)} - v_b G_{12}^{(1)}) \partial_j (A_j^{-1} A_{3-j} \partial_j ()) - (G_{12}^{(1)} - v_b G_{11}^{(1)}) \partial_{3-j} (A_j A_{3-j}^{-1} \partial_{3-j} ()) \right\},
\end{aligned}$$

$$j, l = 1, 2, \quad \rho = 2 - \delta_{jl}, \quad s = 1 + \delta_{jl},$$

$$p_{33} = \frac{v_b (G_{11}^{(1)} + G_{12}^{(1)})}{E_b} \Delta - \frac{v_b (G_{11}^{(0)} + G_{12}^{(0)}) (k_1 + k_2)}{E_b},$$

$$p_{34} = -\frac{4}{A_1 A_2} \frac{1 + v_b}{E_b} G_{66}^{(1)} (\partial_1 \partial_2 + \partial_1 (\xi_{10}^1 ()) + \partial_2 (\xi_{10}^2 ())).$$

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