Analysis and design of thermo-mechanical interfaces

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Abstract. An elastic structure subjected to thermal and mechanical loading with prescribed external boundary and varying internal interface is considered. The different thermal and mechanical nature of this interface is discussed, since the interface form and its properties affect strongly the structural response. The first-order sensitivities of an arbitrary thermal and mechanical behavioral functional with respect to shape and material properties of the interface are derived using the direct or adjoint approaches. Next the relevant optimality conditions are formulated. Some examples illustrate the applicability of proposed approach to control the structural response due to applied thermal and mechanical loads.

Key words: multiphase structures, sensitivity analysis, optimization, heat transfer, thermo-elasticity.

1. Introduction

Recently, there has been a great deal of interest in methods of calculating the sensitivity of global behavioral response or local quantities with respect to shape and material variations for a wide class of boundary-value problems. The present paper constitutes an extension of previous author's works in this area [1–9]. The multi-phase structure can be subjected to purely thermal or mechanical or combined thermo-mechanical boundary conditions and the variation of an arbitrary thermal or mechanical functional describing the structural quality is considered with respect to shape of interface separating the different phases of structural material. The nature of this interface influences the structural response due to thermal, mechanical or thermo-mechanical service load. The fundamental analysis of multiphase thermomechanics with presence of interfaces was presented by Gurtin [10, 11] next by Angenent and Gurtin [12] for evolving plane interfaces. The numerical study of transient thermomechanical states in two-phase materials was presented by Furukawa et al. [13] by applying the boundary element method. The interphase model between two elastic materials treated as a thin conducting layer was discussed by Ivanova et al. [14].

In deriving the desired sensitivities of considered functional, both the direct and/or adjoint approaches can be used. The direct approach is based on specification of sensitivity derivatives of state fields, while the concept of adjoint systems with introduced adjoint structure associated with the considered functional will be applied in the adjoint method. The obtained sensitivity expressions can be utilized in analyzing the structural behavior associated with small variation of interface shape and location within structural domain, or can be used in formulating the relevant optimality conditions for the assumed optimal design problem. An arbitrary behavioral functional can be taken as objective function with account

for design constraints. The present analysis is confined to the geometrically linear theory, assuming thermally anisotropic material and nonlinear stress-strain relations. However, generalization to geometrically nonlinear behavior of a structure will be possible by following the presented analysis.

2. Formulation of problem

In this paper we shall discuss the sensitivity analysis of an arbitrary objective functional representing the measure of quality for a composite multi-phase structure and next the optimal design of such structure, for which the internal interface separating these phases can undergo some assumed shape modification, as shown in Fig. 1. The material properties of this interface can be also modified during optimization process. The key point of any gradient oriented optimization algorithm is the sensitivity analysis of arbitrary thermal and mechanical functionals defined within a domain of structure, associated with particular optimization problem. The shape variation of structural domain Ω associated with internal boundary modification can be defined as an infinitesimal transformation process

$$\Omega \Rightarrow \Omega^t : \mathbf{x}^t = \mathbf{x} + \delta\boldsymbol{\varphi}(\mathbf{x}, \mathbf{b}) = \mathbf{x} + \mathbf{v}^p(\mathbf{x}, \mathbf{b})\delta b_p, \quad (1)$$

where the transformation field $\boldsymbol{\varphi}(\mathbf{x},\mathbf{b})$ is a given function of space position and depends on a set $\mathbf{b}$ of independent design parameters b_p , $p=1,2,...P$, and $\mathbf{v}^p(\mathbf{x}, \mathbf{b}) = \partial\boldsymbol{\varphi}(\mathbf{x}, \mathbf{b})/\partial b_p$ denotes a transformation velocity field associated with shape parameter b_p treated as time-like parameter. Such description of domain modification allows us to use the material derivative (or rate) concept in deriving the desired sensitivities of considered functional.

An interface Γ_s, shown in Fig. 1, can represent here either the internal surface separating two materials with different thermal and mechanical properties or can be treated as

a discrete material surface inclusion of vanishing thickness with the properties different than the properties of material of structure. The latter interface can be regarded as surface on which some thermal and mechanical state fields undergo discontinuities.
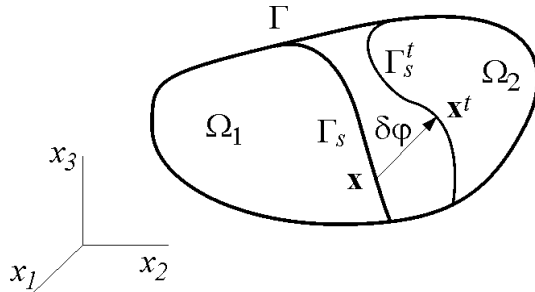

Fig. 1. A structure occupying domain Ω with varying interface Γ_s

The behavior of structure subjected to thermal and/or mechanical loads can be described by the sets of equations describing heat transfer within structure domain and mechanical response due to applied load.

Let us define first the heat conduction problem, which is governed by the following set of equations:

$$\operatorname{div}\mathbf{q} - Q = 0, \quad \mathbf{q} = -\mathbf{A} \cdot \nabla T + \mathbf{q}^i \quad \text{in} \quad \Omega,$$
$$T = T^0 \quad \text{on} \quad \Gamma_T, \quad q_n = q_{n0} \quad \text{on} \quad \Gamma_q,$$
$$q_n = k_c(T - T_\infty) \quad \text{on} \quad \Gamma_h, \tag{2}$$
$$\text{and additional conditions on} \quad \Gamma_s,$$

where T and $\mathbf{q}$ denote the temperature field and heat flux vector, $\mathbf{A}$ and k_c denote the anisotropic material conductivity matrix and convection coefficient, respectively, and T_∞ denotes the surrounding temperature, while $\mathbf{q}^i$ and Q can be regarded as the initial heat flux and heat generation source term within the structure domain. The temperature T^0 is specified on the boundary portion Γ_T, while the prescribed heat flux q_{n0} is specified on the portion Γ_q and the convection condition is defined on Γ_h. The additional conditions on interface Γ_s that should be satisfied by state fields T and $\mathbf{q}$, is specified in the next section.

In practical applications the structural analysis is quite often performed using the computer-oriented finite element packages. In this case, instead of description (2), its equivalent matrix formulation can be used, namely:

$$\mathbf{K}_t \mathbf{T} = \mathbf{F}_t \quad \text{and additional conditions on} \quad \Gamma_s, \tag{3}$$

where now $\mathbf{K}_t$ denotes the global conductivity matrix of a structure, $\mathbf{T}$ is a vector of nodal temperatures of the finite element model of structure and $\mathbf{F}_t = \mathbf{F}_{tq_n} + \mathbf{F}_{tQ} + \mathbf{F}_{t\mathbf{q}^i}$ denotes the vector of nodal thermal forces, yielding by external heat flux as well as internal heat source and initial heat flux applied to the structure, respectively.

In the second case, when the mechanical behavior of structure is considered, it is described by a set of equations defining the following elastic boundary-value problem:

$$\operatorname{div}\boldsymbol{\sigma} + \mathbf{f} = 0, \quad \varepsilon = \frac{1}{2}(\nabla\mathbf{u} + \nabla^T\mathbf{u}) \quad \text{in} \quad \Omega,$$
$$\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t}^0 \quad \text{on} \quad \Gamma_t, \quad \mathbf{u} = \mathbf{u}^0 \quad \text{on} \quad \Gamma_u, \tag{4}$$
$$\boldsymbol{\sigma} = \mathbf{S}(\varepsilon, \boldsymbol{\sigma}^i),$$
$$\text{and additional conditions on} \quad \Gamma_s,$$

where $\boldsymbol{\sigma}$, $\boldsymbol{\varepsilon}$ and $\mathbf{u}$ denote the stress, strain and displacement fields, respectively, $\mathbf{f}$ denotes a body force field while $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n}$ is a traction vector and the last equation of (4) defines nonlinear stress-strain relation. The initial stress field caused by temperature field within a structure is denoted by $\boldsymbol{\sigma}^i$. Moreover, Γ_t and Γ_u denote here the boundary portions, on which the tractions $\mathbf{t}^0$ and displacement $\mathbf{u}^0$ are prescribed. The additional conditions on interface Γ_s will be also specified in the following section.

Similarly as before, when in practical applications the finite element approach to structural analysis is used, the equivalent for Eqs. (4) can be written in the form:

$$\mathbf{K}_m \mathbf{u} = \mathbf{F}_m \quad \text{and additional conditions on} \quad \Gamma_s. \tag{5}$$

Here, $\mathbf{K}_m$ denotes the global stiffness matrix of a structure, $\mathbf{u}$ is a vector of nodal displacements of finite element model of structure and $\mathbf{F}_m = \mathbf{F}_{m\mathbf{t}} + \mathbf{F}_{m\mathbf{f}} + \mathbf{F}_{m\sigma^i}$ denotes the vector of nodal forces, yielding by surface tractions, body forces and initial stresses applied to the structure, respectively.

3. Classification of interfaces

In order to define correctly the boundary-value problems (2) and (4) or (3) and (5), introduced in the previous section, we have to classify the types of thermal and mechanical interfaces within the structure domain and formulate the additional conditions that have to be satisfied by state fields along each particular interface.

Consider first the interface separating materials with different thermal or/and mechanical properties. For the thermal response of structure, the continuity of temperature and normal heat flux across interface is assured, so that:

$$\langle T \rangle = 0, \quad \langle q_n \rangle = \mathbf{n} \cdot \langle \mathbf{q} \rangle = 0 \quad \text{on} \quad \Gamma_s, \tag{6}$$

where $\langle . \rangle$ denotes the discontinuity of the enclosed quantity. Let us note that no other additional conditions along interface for both formulations (2) and (3) should be introduced. Then mechanical response of structure is also characterized in this case by continuity of displacements and internal tractions along interface, that is

$$\langle u \rangle = 0, \quad \langle \mathbf{t} \rangle = \langle \sigma \rangle \cdot \mathbf{n} = 0 \quad \text{on} \quad \Gamma_s \tag{7}$$

with no additional conditions along interface for continuous and discrete formulations (3) and (5), respectively.

More difficult conditions appear when the interface constitutes a thin inclusion surface with different thermal and/or mechanical properties than the material of structure. Consider first the thermal behavior of structure. When the conductivity coefficient of interface is considerably smaller than the coefficients of structural material, then the interface can be

considered as *isolating* surface on which the discontinuity of temperature fields occurs, however, the continuity of normal heat flux is preserved, cf. Fig. 2. The normal heat flux is assumed to be proportional to jump of temperature across the interface. Thus, the following conditions have to be satisfied on Γ_s:

$$\langle T \rangle \neq 0, \quad \langle q_n \rangle = \mathbf{n} \cdot \langle \mathbf{q} \rangle = 0,$$
$$q_n = k_r \langle T \rangle \quad \text{on} \quad \Gamma_s, \tag{8}$$

where k_r denotes the coefficient of thermal resistance of the interface material.
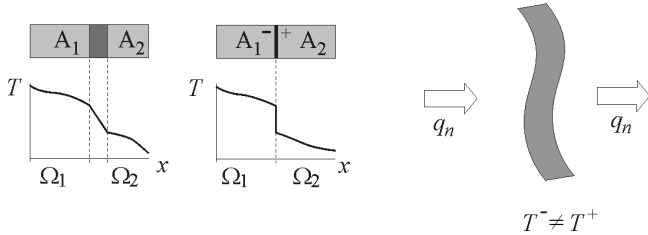

Fig. 2. Model of thermally isolating interface

On the other hand, when the conductivity of interface is considerably greater than the conductivity of structural material, then the interface plays the role of *conductor* transferring heat along its surface. In this case, the continuity of temperature field across the interface is assumed, whereas the normal flux is allowed to suffer discontinuity and its jump is governed by conduction equation within interface plane or line, cf. Fig. 3. Thus, the thermal state fields should satisfy the following conditions:

$$\langle T \rangle = 0, \quad \langle q_n \rangle \neq 0, \quad \text{div}_\Gamma \widehat{\mathbf{q}} = \langle q_n \rangle,$$
$$\widehat{\mathbf{q}} = -\widehat{\mathbf{A}} \cdot \nabla_\Gamma T \quad \text{on} \quad \Gamma_s, \tag{9}$$

where $\widehat{\mathbf{q}}$ and $\widehat{\mathbf{A}}$ denote the heat flux vector and the conductivity matrix within the interface. The last two equations of (7) describe thus the heat conduction within the interface with the jump of normal flux treated as the internal heat generation source.
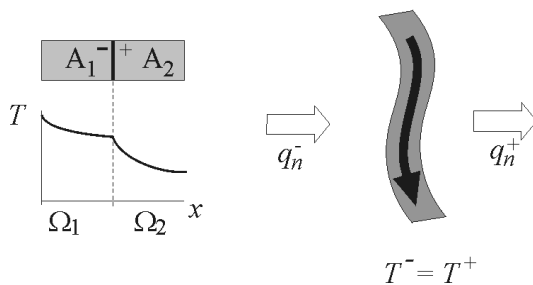

Fig. 3. Model of thermally conducting interface

When the finite element formulation (3) is used in order to analyze the thermal structural response, then some additional one- or two-dimensional resistance or conducting elements have to be introduced along interface surface or line, respectively.

A similar behavior of the interface inclusion can be observed for a mechanical system. Depending on ratio of stiffness moduli of interface and structural material, the interface

within elastic structure can be considered as *reinforcing* or *softening* surfaces. In the former case, when the interface is stiffer than the rest of material and plays a role of discrete reinforcing surface, cf. Fig. 4, the discontinuity of the internal traction vector is observed, whereas the displacement field retains continuity. Thus, we have:

$$\langle \mathbf{u} \rangle = 0, \quad \langle \mathbf{t} \rangle = \langle \sigma \rangle \cdot \mathbf{n} \neq 0 \quad \text{on} \quad \Gamma_s. \tag{10}$$
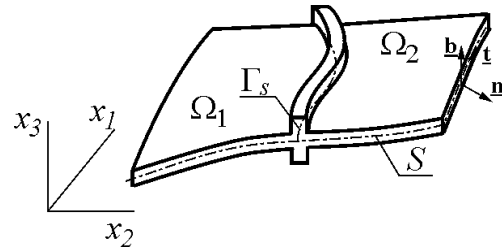

Fig. 4. Reinforcing interface

The jump in internal forces is related to the generalized stresses σ within reinforcement through the equilibrium equation. On the other hand, for a weak or softening interface (in mechanical sense), cf. Fig. 5, the discontinuity of displacements can be assumed. On the surface, however, preserving the continuity of internal tractions which are assumed to be proportional to the jump in displacements across the interface, that is:

$$\langle \mathbf{u} \rangle \neq 0, \quad \langle \mathbf{t} \rangle = 0, \quad \mathbf{t} = \mathbf{C} \cdot \langle \mathbf{u} \rangle \quad \text{on} \quad \Gamma_s, \tag{11}$$

where $\mathbf{C}$ is a matrix of stiffness coefficients along interface and $\langle \mathbf{u}^i \rangle$ denotes the jump of displacements on both sides of interface. The detailed analysis of such mechanical system with strong discontinuities of static and kinematic fields was presented in [3–5].
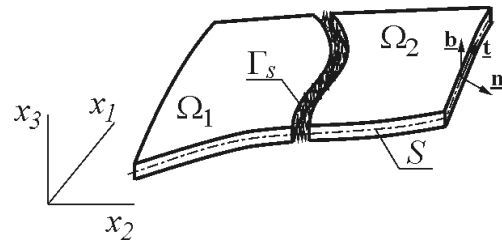

Fig. 5. Softening interface

When, similarly as for thermal case, the finite element formulation (5) is used in order to analyze the mechanical structural response, then some additional finite elements have to be introduced along interface surface or line, respectively. The curvilinear beam or shell elements have to be added to the finite element model of structure in the case of reinforcing interface, while for softening one the slip or hinge elements with or without friction possibilities should be added.

Considering now simultaneously the thermo-mechanical system with the interfaces discussed above, we obtain the wide class of different thermal and mechanical structural behavior due to particular properties of interface. The possible combinations of thermal and mechanical properties of an interface are shown in Table 1.

Table 1
Possible classes of interfaces

	Mechanical properties of the interface		
Thermal conductivity of interface	weak {Eq.(11)}	strong {Eq.(10)}	separating interface {Eq.(7)}
small {Eq.(8)}	isolating softening surface	isolating reinforcing surface	isolating & mechanically separating surface
great {Eq.(9)}	conducting softening surface	conducting reinforcing surface	conducting & mechanically separating surface
separating interface {Eq.(6)}	thermally separating softening surface	thermally separating reinforcing surface	thermally & mechanically separating surface

Thus, it can be seen that playing with thermal and mechanical properties of structural interface, we can influence the thermal and mechanical response of structure. Moreover, changing the shape or material properties of the interface we can also design the structural configuration and material, in order to obtain its desired response.

4. Thermal and mechanical response functionals

Let us now define arbitrary thermal and mechanical behavioral functionals which can play the role of objective functional or global constraint in a design or the optimization procedure. The thermal functional can be assumed in the form:

$$G_t = \int \Psi_t(T, \nabla T, \mathbf{q}) d\Omega$$
$$+ \int \Phi_t(T, q_n) d\Gamma + \int \widehat{\Phi}_t d\Gamma_s, \tag{12}$$

where $\widehat{\Phi}_t = 0$ for the case of separating interface, $\widehat{\Phi}_t = \widehat{\Phi}_t(\overline{T}, \langle T \rangle, q_n)$ for the case of structure with isolating interface and $\widehat{\Phi}_t = \widehat{\Phi}_t(T, \overline{q}_n \langle q_n \rangle)$ when the conducting interface appears within structure domain. $\overline{T}$ and $\overline{q}_n$ denote here the average temperature and normal heat flux, respectively. On the other hand, the mechanical behavioral functional can be considered in the form:

$$G_m = \int \Psi_m(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}, \mathbf{u}, \sigma^i) d\Omega$$
$$+ \int \Phi_m(\mathbf{t}, \mathbf{u}) d\Gamma + \int \widehat{\Phi}_m d\Gamma_s, \tag{13}$$

where now $\widehat{\Phi}_m = 0$ for the case of separating interface, $\widehat{\Phi}_m = \widehat{\Phi}_m(\langle \mathbf{t} \rangle, \mathbf{u}, \overline{\boldsymbol{\sigma}}^i)$ for structure with reinforcing interface and $\widehat{\Phi}_m = \widehat{\Phi}_m(\mathbf{t}, \langle \mathbf{u} \rangle, \overline{\mathbf{u}}^i)$ in the case of structure with softening interface. In two last cases $\overline{\boldsymbol{\sigma}}^i$ and $\overline{\mathbf{u}}^i$ denote the imposed fields of initial stress and initial displacement on reinforcing and softening interfaces, respectively.

5. Sensitivity analysis for response functionals

Our first goal is now to derive the first-order sensitivities of functionals (12) and (13) with respect to variation of shape design parameters b_p defining the shape of interface within the structure domain. Differentiating (12) and (13) with respect to b_p, we get:

$$\frac{DG_t}{Db_p} = \int \left[\frac{D\Psi_t}{Db_p} d\Omega + \Psi_t \frac{D(d\Omega)}{Db_p} \right]$$
$$+ \int \left[\frac{D\Phi_t}{Db_p} d\Gamma + \Phi_t \frac{D(d\Gamma)}{Db_p} \right] \tag{14}$$
$$+ \int \left[\frac{D\widehat{\Phi}_t}{Db_p} d\Gamma_s + \widehat{\Phi}_t \frac{D(d\Gamma_s)}{Db_p} \right]$$

and

$$\frac{DG_m}{Db_p} = \int \left[\frac{D\Psi_m}{Db_p} d\Omega + \Psi_m \frac{D(d\Omega)}{Db_p} \right]$$
$$+ \int \left[\frac{D\Phi_m}{Db_p} d\Gamma + \Phi_m \frac{D(d\Gamma)}{Db_p} \right] \tag{15}$$
$$+ \int \left[\frac{D\widehat{\Phi}_m}{Db_p} d\Gamma_s + \widehat{\Phi}_m \frac{D(d\Gamma_s)}{Db_p} \right],$$

where the sensitivities of integrands on the right-hand sides of (14) and (15) can be expressed explicitly in terms of design parameters.

Performing the sensitivity analysis with respect to shape and thermal or mechanical properties of interfaces, the similar approach as in the case of sensitivity analysis for structure with varying external boundary can be used. As it is shown in Fig. 6, the domain of the structure with the fixed external boundary and varying interface can be considered as a sum of two or three subdomains with partially varying external boundaries and then the sensitivity expressions obtained earlier for the case of varying external boundary can be applied to the case of varying interface. In fact, the functionals G_t (14) and G_m (15) can be rewritten in the form:

$$G_t = G_t^1 + G_t^2 + G_t^3,$$
$$G_m = G_m^1 + G_m^2 + G_m^3 \tag{16}$$

and then the sensitivities (14) and (15) can be expressed as:

$$\frac{DG_t}{Db_p} = \frac{DG_t^1}{Db_p} + \frac{DG_t^2}{Db_p} + \frac{DG_t^s}{Db_p}$$
$$\frac{DG_m}{Db_p} = \frac{DG_m^1}{Db_p} + \frac{DG_m^2}{Db_p} + \frac{DG_m^s}{Db_p}. \tag{17}$$

The particular form of above expressions can be obtained using the direct or adjoint approaches. The detailed sensitivity analysis for the base case of external boundary variation and next internal separating surface modification for thermal system was presented in [1, 6], whereas the case of varying isolating and conducting interfaces was discussed in details in [7].

Similarly, the sensitivity analysis for the case of mechanical system was presented in [3–5]. Therefore, in the present paper we recall only the proper sensitivity expressions and next apply them in optimality conditions derived in the next section.
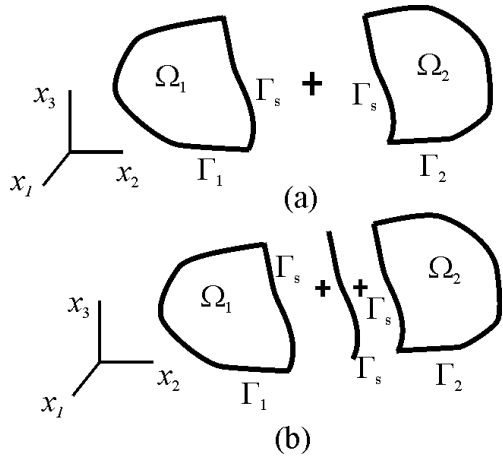

Fig. 6. Decomposition of structure with separating interface (a) and surface inclusion (b)

Applying the direct method of sensitivity analysis to thermally loaded structure, we differentiate the heat transfer equations (2) with respect to each design parameter, constructing in this way P additional heat transfer problems with state fields $T_{,p}$ and $\mathbf{q}_{,p}$ being the local (for fixed structural shape) sensitivities of primary temperature and heat flux fields. These additional heat transfer problems are described by the following set of equations:

$$\operatorname{div}\mathbf{q}_{,p} - Q_{,p} = 0, \quad \mathbf{q}_{\cdot p} = -\mathbf{A}\cdot\nabla T_{,p} + \mathbf{q}^{pi} \quad \text{in} \quad \Omega,$$
$$T_{,p} = T^{p0} \quad \text{on} \quad \Gamma_T, \quad q_{n,p} = q^p_{n0} \quad \text{on} \quad \Gamma_q, \qquad (18)$$
$$q_{n,p} = k_c(T_{,p} - T^p_\infty) \quad \text{on} \quad \Gamma_h,$$

with proper conditions on interface Γ_s following from differentiation of interface conditions (6), (8) or (9). When the finite element approach is used in analyzing the thermal behavior of structure, the description of additional heat transfer problems follows from differentiation of (3) and takes the form:

$$\mathbf{K}_t\mathbf{T}^p = \mathbf{F}^p_t,$$
$$\mathbf{T}^p = \mathbf{T}_{,p} \quad , \quad \mathbf{F}^p_t = \mathbf{F}_{t,p} - \mathbf{K}_{t,p}\mathbf{T}, \qquad (19)$$

where $\mathbf{F}^p_t$ denote now the vector of additional nodal thermal forces. Solving Eqs. (18) or (19) the local derivatives of temperature and heat flux fields are derived and next the desired sensitivities of thermal response functional (12) can be calculated.

Considering, for instance, the varying conducting interface specified by conditions (9), the sensitivity expression $(16)_1$ for thermal functional takes the final form, cf. [7]:

$$\frac{DG_t}{Db_p} = \int (\Psi_{t,T}\,T_{,p} + \nabla_{\nabla T}\Psi_t\cdot\nabla T_{,p} + \nabla_q\Psi_t\cdot\mathbf{q}_{,p})d\Omega$$
$$+ \int \Phi_{t,T}T_{,p}\,d\Gamma_q + \int \Phi_{t,q_n}\,q_{n,p}\,d\Gamma_t$$
$$+ \int (\Phi_{t,T} + k_c\Phi_{t,q_n})\,T_{,p}\,d\Gamma_h$$
$$+ \int \left[\left(\langle\Psi_t\rangle - 2H\widehat{\Phi}_t\right)\mathbf{n} - \nabla_\Gamma\widehat{\Phi}_t\right]\cdot\mathbf{v}^p d\Gamma_s \qquad (20)$$
$$+ \int \left[\widehat{\Phi}_{t,T}\left(T_{,p} + \nabla T\cdot\mathbf{v}^p\right)\right.$$
$$\left. + \widehat{\Phi}_{t,\langle q_n\rangle}\left(\langle q_{n,p}\rangle + \langle\nabla q_n\rangle\cdot\mathbf{v}^p - \langle\mathbf{q}_\Gamma\rangle\cdot\nabla_\Gamma v^p_n\right)\right]d\Gamma_s,$$
$$p = 1, 2, \dots, P,$$

where H denotes the mean curvature of interface Γ_s, ∇_Γ is the tangent gradient operator and $\mathbf{q}_\Gamma$ denotes the tangent heat flux.

When the adjoint approach to sensitivity analysis for the thermal case is applied, one has to introduce the only one adjoint heat transfer problem with heat source, initial heat flux and boundary conditions depending on the form of behavioral functional G_t. Denoting the adjoint state fields by T^a and $\mathbf{q}^a$, the adjoint problem is described by the following set of equations:

$$\operatorname{div}\mathbf{q}^a - Q^a = 0, \quad \mathbf{q}^a = -\mathbf{A}\cdot\nabla T^a + \mathbf{q}^{ai} \quad \text{in} \quad \Omega,$$
$$T^a = T^{a0} \quad \text{on} \quad \Gamma_T, \quad q^a_n = q^a_{n0} \quad \text{on} \quad \Gamma_q, \qquad (21)$$
$$q^a_n = k_c(T^a - T^a_\infty) \quad \text{on} \quad \Gamma_h$$

with proper conditions on interface Γ_s, similar to those specified for primary system. The finite element formulation of the adjoint problem is similar to (3) and can be written as follows:

$$\mathbf{K}_t\mathbf{T}^a = \mathbf{F}^a_t,$$
$$\mathbf{F}^a_t = \mathbf{F}^a_{tq_n} + \mathbf{F}^a_{tQ} + \mathbf{F}^a_{t\mathbf{q}^{ai}}, \qquad (22)$$

where $\mathbf{F}^a_t$ denotes now the vector of additional nodal thermal forces. Solving Eqs. (21) or (22) the adjoint temperature and heat flux fields are derived and next the desired sensitivities of thermal response functional (12) can be calculated.

Considering, for instance, the varying separating interface specified by conditions (6), the sensitivity expression $(17)_1$ for thermal functional takes now the final form:

$$\frac{DG_t}{Db_t} = \int \left[\left(\langle\Psi_t\rangle - \langle T_{,n}\rangle q^a_n + \langle q_{n,n}\rangle T^a\right)v^p_n\right.$$
$$\left. - T^a\langle\mathbf{q}_\Gamma\rangle\cdot\nabla_\Gamma v^p_n\right]d\Gamma_s, \qquad (23)$$
$$p = 1, 2, \dots, P.$$

In the case of isolating interface specified by conditions (8), the above approach yields the following sensitivity expression:

$$\frac{DG_t}{Db_t} = \int \left\{\left[\left(\langle\Psi_t\rangle - 2H\widehat{\Phi}_t\right)\mathbf{n}\right.\right.$$
$$\left.\left. + \left(\widehat{\Phi}_{t,\langle T\rangle} - \rho\widehat{\Phi}_{t,q_n}\right)\langle\nabla T\rangle - \nabla_\Gamma\widehat{\Phi}_t\right]\right. \qquad (24)$$
$$\left. \cdot\mathbf{v}^p - \langle T^a\mathbf{q}_\Gamma\rangle\cdot\nabla_\Gamma v^p_n\right\}d\Gamma_s,$$
$$p = 1, 2, \dots, P.$$

The similar expressions can be also easily obtained for the case of elasticity problem, using both the direct or adjoint approaches. Limiting ourselves to adjoint sensitivity method, an adjoint elasticity problem with boundary conditions depending on the form of mechanical functional (13) has to be solved, yielding the adjoint displacement, strain and stress fields $\mathbf{u}^a$, $\boldsymbol{\varepsilon}^a$ and $\boldsymbol{\sigma}^a$, respectively. This adjoint boundary value problem has the form similar to (4) and it is described by the equation set of the form:

$$\operatorname{div}\boldsymbol{\sigma}^a + \mathbf{f}^\alpha = 0, \quad \boldsymbol{\varepsilon}^a = \frac{1}{2}(\nabla\mathbf{u}^a + \nabla^T\mathbf{u}^a) \quad \text{in} \quad \Omega,$$
$$\boldsymbol{\sigma}^a \cdot \mathbf{n} = \mathbf{t}^{a0} \quad \text{on} \quad \Gamma_t, \quad \mathbf{u}^a = \mathbf{u}^{a0} \quad \text{on} \quad \Gamma_u, \qquad (25)$$
$$\boldsymbol{\sigma}^a = \mathbf{D}(\boldsymbol{\varepsilon}^a - \boldsymbol{\varepsilon}^{ai}) - \boldsymbol{\sigma}^{ai},$$

supplemented with proper conditions on interface Γ_s similar to those specified for primary system and given by (7), (10) or (11). Considering first the varying separating interface specified by conditions (7), the sensitivity expression $(17)_2$ for mechanical functional takes the final form:

$$\frac{DG_m}{Db_t} = \int \left(\langle\Psi_m\rangle - \langle\sigma\cdot\varepsilon^a\rangle + \mathbf{t}\cdot\langle\mathbf{u},_n^a\rangle \right.$$
$$\left. +\mathbf{t}^a\cdot\langle\mathbf{u},_n\rangle \right) v_n^p d\Gamma_s, \qquad p = 1,2,\ldots,P. \qquad (26)$$

In the case of reinforcing interface shown in Fig. 4 and specified by conditions (10), given in the form of reinforcing fiber of curvature K, the adjoint approach yields the sensitivity expressions in the form:

$$\frac{DG_m}{Db_t} = \int \left(\langle\Psi_m\rangle - \widehat{\Phi}_m K - \langle\sigma_{ss}\rangle\varepsilon_{ss}^a + \langle\sigma_{ns}\varepsilon_{ns}^a\rangle \right.$$
$$\left. +\langle\sigma_{nn}^a\varepsilon_{nn}\rangle - N\kappa^a - N^a\kappa - N^a\varepsilon K \right) v_n^p d\Gamma_s, \qquad (27)$$
$$p = 1,2,\ldots,P,$$

where (n, s) denotes the local coordinate system along reinforcing line and N, ε, κ are the normal force, elongation and curvature in reinforcing fiber, respectively. Finally, considering the softening interface shown in Fig. 5, given in the form of softening line separator of curvature K, the sensitivity expressions $(17)_2$ for functional (13), obtained by using adjoint approach, can be specified as:

$$\frac{DG_m}{Db_t} = \int \left[\langle\Psi_m\rangle - \widehat{\Phi}_m K - \langle\boldsymbol{\sigma}\cdot\boldsymbol{\varepsilon}^a\rangle \right.$$
$$+t_{n\alpha}\langle u_{n\alpha}^a\rangle K - t_{n\alpha}\langle u_{\alpha,n}^a\rangle$$
$$\left. +e_{3\alpha\beta}(t_{n\alpha}\langle u_\beta^a\rangle + t_{n\alpha}^a\langle u_\beta\rangle),_s \right] v_n^p d\Gamma_s, \qquad (28)$$
$$\alpha,\beta = n, s, \qquad p = 1,2,\ldots,P,$$

where, as before, (n, s) denotes the local coordinate system along discontinuity line.

6. Optimality conditions

The typical optimization problem can be stated, for instance, as minimizing the thermal objective functional (12) subjected to mechanical and cost constraints, and can be written as follows:

$$\text{minimize } G_t \text{ subject to } \begin{cases} G_m - G_m^0 \le 0, \\ C - C_0 \le 0, \end{cases} \qquad (29)$$

where G_m^0 denotes the upper bound on global mechanical behavioral constraint, $C = \int c d\Omega$ is a structural cost and C_0 denotes the upper bound on the cost of structure.

Let us assume that the problem (29) is concerned with the structure containing the thermally isolating and mechanically reinforcing interface within its domain. In this case, the jump in temperature along interface can induce significant initial thermal stresses and then the global mechanical constraint should be mainly imposed on effective stresses in order to assure the safe response of optimal structure under service load. When the isolating interface behaves as mechanically softening inclusion, then it can cause the desired thermal response, preserving at the same time the proper redistribution of induced thermal stresses, according to the form of imposed mechanical constraint. On the other hand, assuming the structure with thermally conducting interface, the induction of initial thermal stresses in interface can be avoided, due to continuity of temperature field across this interface, and the mechanical constraint in (29) can not affect essentially the optimal structure response.

The other possible optimization formulation can be focus on minimization of a proper mechanical functional (13) with constraints put on structural cost and thermal behavior of structure. In this case the optimal design problem can be stated as:

$$\text{minimize } G_m \text{ subject to } \begin{cases} G_t - G_t^0 \le 0, \\ C - C_0 \le 0, \end{cases} \qquad (30)$$

Also the weighted functional can be used as objective goal in optimization procedure with global constraint put on structural cost, namely:

$$\text{minimize } G = \alpha_t G_t + \alpha_m G_m \text{ subject to } C - C_0 \le 0. \quad (31)$$

The optimality conditions for any kind of optimization problem follow from the stationarity of Lagrange functional. For instance, for the problem (30), they take the form:

$$\frac{DG_m}{Db_p} + \xi_1\frac{DC}{Db_p} + \xi_2\frac{DG_t}{Db_p} = 0,$$
$$C - C_0 + \eta_1^2 = 0, \qquad 2\xi_1\eta_1 = 0, \qquad (32)$$
$$G_t - G_t^0 + \eta_2^2 = 0, \qquad 2\xi_2\eta_2 = 0,$$

where ξ_1 and ξ_2 are the Lagrange multipliers and η_1 and η_2 denote slack variables. The sensitivities DG_t/Db_p and DG_m/Db_p appearing in optimality conditions are derived following the sensitivity analysis already discussed in previous section. The similar conditions can be easily obtained for the optimization problem (29) or (31).

7. Illustrative examples

In order to illustrate the applicability of proposed approach some simple examples of optimal shape design of thermal and mechanical interfaces within structure domain were analyzed and will be discussed here. Two first examples concern the problem of heat transfer within structure domain, whereas

the two last examples are related to mechanical behavior of structure.

Example 1. This example is related to the heat conduction problem in two-phase disk with fixed internal hole and external boundary and varying interface separating two isotropic materials of different thermal properties, cf. Fig. 7. The varying interface separating domains Ω_1 and Ω_2 is composed either from 8 piecewise linear parts with two independent design parameters a_1, a_2, as shown in Fig. 7a, or forms a rectangle which sides can undergo translations a_1 and a_2, cf. Fig. 7b. Assuming the convection boundary condition along hole boundary and prescribed temperature along external boundary, consider the functional representing the amount of heat transfer through the external disk boundary, given in the form:

$$G_t = \int_{\Gamma_e} q_n d\Gamma_e \qquad (33)$$

and determine the optimal forms of interface for both possible modifications shown in Fig. 7a and b, respectively, assuming the constant area $\widehat{A}_1$ of domain Ω_1.
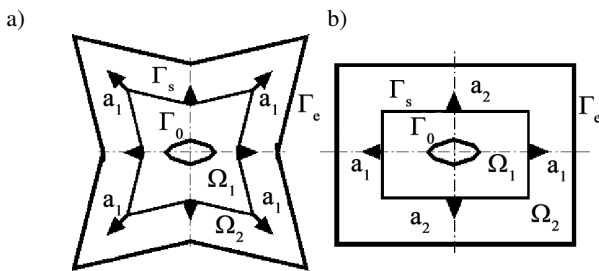

Fig. 7. Disk with varying piece-wise linear (a) and rectangular (b) interface

Regarding this example as a model of heat isolator with a hole containing a fluid of specified temperature T_0 and transferring the heat through the fixed boundary kept in constant temperature T_e, the optimization problem can be stated as follows:

$$\min_{a_1, a_2} \; G_t \quad \text{subject to} \quad A_1 - \widehat{A}_1 = 0, \qquad (34)$$

where denotes the area of isolating domain and $\widehat{A}_1$ is a prescribed quantity. The optimality conditions follow from stationarity of Lagrange functional and take the form

$$\frac{DG_t}{Db_p} + \xi_1 \frac{DA_1}{Db_p} = 0 \quad \text{for} \quad b_p = a_1, \; a_2,$$
$$A_1 - \widehat{A}_1 = 0, \qquad (35)$$

where ξ_1 is the Lagrange multiplier, DA_1/Db_p denotes the disk area sensitivity and the sensitivities of functional G_t can be calculated using the adjoint approach from expressions (24).

The two-step analysis-synthesis algorithm was applied in order to solve the optimality conditions (35) and to derive the optimal values of design parameters a_1 and a_2. The optimal shapes of disk for some selected particular data $\lambda_1 =$

120.0 W/(m^{0}K), $\lambda_2 = 1.0$ W/(m^{0}K), $h = 240.0$ W/(m^2 ^{0}K), $T_0 = 150°$C, $T_e = 20°$C, and prescribed area $\widehat{A}_1 = 4.0$ m^2, are depicted on Fig. 8 for both possible modification of interface Γ_s. The optimal solutions for assumed data were improved, in comparison to initial design shown with dotted lines in Fig. 8, with 19.7% for shape modification shown in Fig. 8a and with 33.2% for the case of shape modification shown in Fig. 8b.
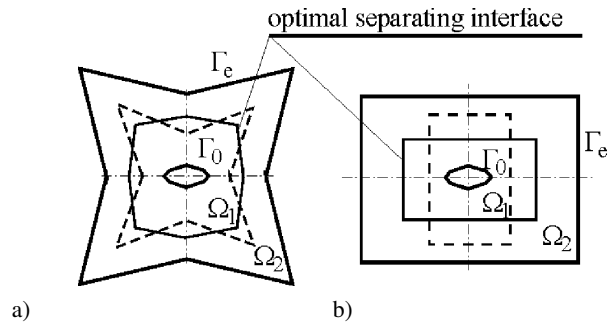

Fig. 8. Optimal shape of quadrilateral (a) and rectangular (b) separating interface in two-phase disk

Example 2. In this second example it was assumed that the disk shown in Fig. 7 is made from isotropic material and contains an isolating layer modeled with a varying isolating interface separating domains Ω_1 and Ω_2. The boundary and initial conditions were assumed to be the same as in previous example. Regarding again this example as a model of heat isolator the optimization problem is formulated again by (34), where now a_1 and a_2 are design parameters determining the shape of isolating interface, as shown in Fig. 7a and b, respectively, and $\widehat{A}_1$ is a prescribed area of domain Ω_1 of a disk. The optimality conditions have the form (35), where the sensitivities of functional G_t appearing in (34) were now calculated from expression (24). Using the solution algorithm similar to that applied in previous examples, the optimization problem (34) was solved for some particular data $\lambda_1 = \lambda_2 = 120$ W/(m^{0}K), $h = 240.0$ W/(m^2 ^{0}K), $k_r = 20$ W/(m^2 ^{0}K), $T_0 = 150°$C, $°$C $T_e = 20$ and $\widehat{A}_1 = 4.0$ m^2. Optimal shapes of interface are shown with solid line in Fig. 9a and b, respectively, while the dotted lines represent the initial design. The decreasing of functional G_t was 16.6% for the case from Fig. 9a when compared to initial design, while the increasing of G_t for the case from Fig. 9b was about 1.1%.
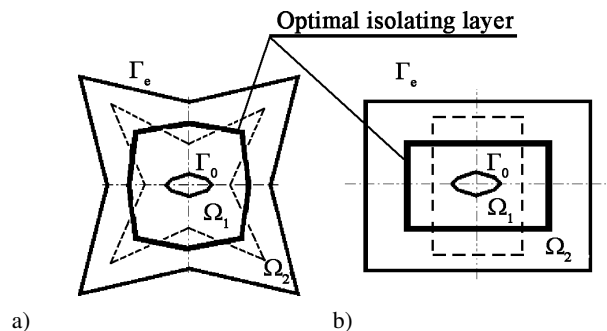

Fig. 9. Optimal shape of quadrilateral (a) and rectangular (b) isolating interface in two-phase disk

Example 3. The axi-symmetrical plate reinforced with closed circular stiffener clamped along external boundary, cf. Fig. 10, is loaded by uniform lateral pressure. The goal of mean stiffness design problem is to find the optimal radius of stiffener within a class of stiffener with its bending rigidity inversely proportional to stiffener length. Thus, the mechanical behavioral functional G_m (13) is selected in the form of potential energy of the plate, given as:

$$\Pi_u = \pi \Bigg\{ D \int\limits_0^{r_e} (\kappa_n^2 + 2\nu\kappa_n\kappa_s + \kappa_s^2$$

$$-pw)rdr + a\kappa_t^2 R \Bigg\} \quad \rightarrow \quad \min.$$

$$\Pi_u = \pi \Bigg\{ D_b \int\limits_0^{r_e} (\kappa_n^2 + 2\nu\kappa_n\kappa_s + \kappa_s^2$$
$$(36)$$

$$-pw)rdr + a\kappa_t^2 R \Bigg\} \quad \rightarrow \quad \min.$$

where D_b denotes the plate stiffness, p, w, κ_n and κ_s are the plate loading, deflection and curvatures, respectively, while a, κ_t and R denote the stiffener rigidity, curvature and radius.
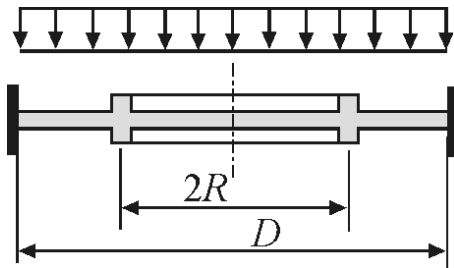

Fig. 10. Clamped plate with circular stiffener

The optimization problem (30) is now stated in the form:

$$\min.\Pi_u \quad \text{subjected to} \quad aR = a_0 r_e = \text{ const.} \quad (37)$$

and the optimality conditions of (37), following from (32) can be written as follows:

$$w_{1,rr} + w_{2,rr} - \frac{2}{R}w_{,r} = 0 \quad (38)$$

yielding the optimal value of stiffener radius:

$$R_{opt} = \frac{\sqrt{2}}{2} r_e. \quad (39)$$

Example 4. In this last example the problem of optimal design of weak separator in a quadrilateral disk with a hole shown in Fig. 11a is considered. The disk is supported along external boundary and loaded with uniform pressure along inner hole boundary. The separator introduces the discontinuity in displacement field along its line and then acts as the softening interface within disk domain, specified by conditions (11). The global measure of local maximal reduced stress was selected as the behavioral functional (13) and the shape of separator in the form of Bezier's curve was described

by six independent design parameters, as shown in Fig. 11b. Thus, the optimization problem was stated as follows:

$$\min.G_\sigma = \left[\frac{1}{A} \int \left(\frac{\sigma_{red}}{\sigma_0} \right)^6 d\Omega \right]^{1/6}$$
$$(40)$$
$$\text{subjected to} \quad l = \int d\Gamma = l_0 = \text{ const.}$$

where A denotes the area of disk, σ_{red} are the reduced stress in disk domain and σ_0 denotes the upper stress limit. For some illustrative data, not specified here, the optimal solution yields the optimal shape of separator for which the local maximal reduced stress was decreased about 57% in comparison to disk without separator and 19% when compared to disk with optimal circular separator. The plot of reduced stress distribution within the disk with optimal shape of separator is depicted in Fig. 12.
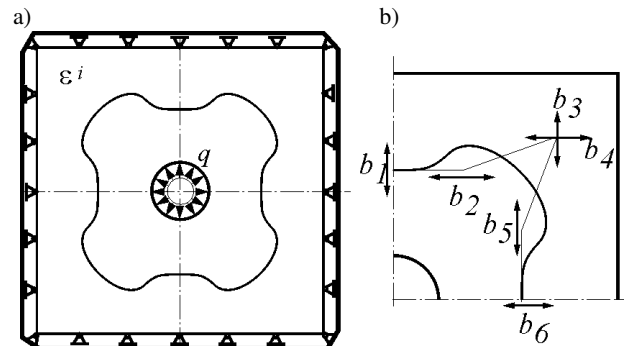

Fig. 11. Quadrilateral disk with separator, (a), and design parameters for Bezier's curve, (b).
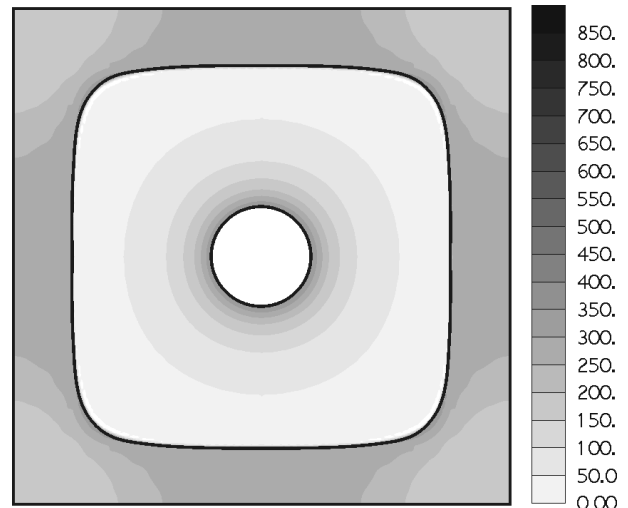

Fig. 12. Reduced stress distribution in disk with optimal separator

8. Concluding remarks

In the present work a sensitivity analysis and optimal design of varying thermo-mechanical interface within structural domain were considered. A systematic approach to direct and adjoint methods of sensitivity analysis was presented and relevant optimality conditions for different objective functionals

based on thermal or mechanical behavioral functionals were derived.

The discussed methods provide effective tools for analyzing any thermo-mechanical system and global response changes with respect to changes of its parameters as well as for generating shapes of interface and its material properties in optimal design, redesign or identification problems.

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