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Optimization of functionally gradient materials under cyclic thermal and mechanical loading

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Abstract

The robust and simple optimization method of FGM is proposed for combined cyclic thermal and mechanical loading.

The optimization procedure starts from the homogeneous ceramic material distribution and after thermomechanical analysis of the whole process, the new distribution of material is determined by reducing concentration of the ceramic phase at places of high tensile stresses and by increasing ceramic contents at places of high effective stresses. The optimal distribution of ceramic phase is found through iterations. The proposed method shares merits of standard optimization and topology optimization because it allows for creation of one phase of material inside the other.

The numerical examples show application of the proposed method to optimization of composite exhaust valve of combustion engine. Examples provided illustrate the optimal density distribution of ceramic phase of Al_2O_3 within $NiAl$ matrix. The transient analysis of stress and temperature fields is used in the design study. The proposed method can be especially useful to problems of structural elements subjected to thermo-mechanical loading histories.

1 Introduction

Thermal stresses play a crucial role in many areas of engineering. In some of engineering structures like car engines, turbine blades, aerospace structures, energy conversion systems, which work in high and non-uniform temperature fields, design of the thermal resistant structures is of primary importance. Ceramic materials, because of their excellent properties at high temperatures and good wear resistance, are currently viewed as promising materials for thermal coatings. However, properties of ceramic coating usually differ from those of the corresponding bulk materials. The difference of thermal expansion coefficient between ceramic coating and bulk

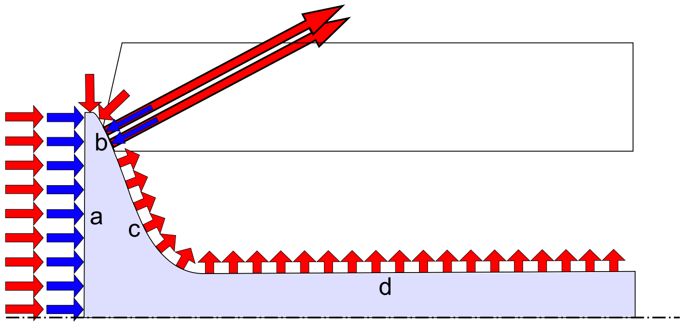


Figure 1: The schematic representation of the axisymmetric valve model used in the finite element simulations. The valve is subjected to mechanical loading at interfaces a (pressure) and b (contact with the engine), while thermal fluxes act at interfaces a, b, c, and d (marked with red colour).

material leads, in case of temperature loading, to high thermal stresses at their interfaces. In order to minimize stress concentration at interfaces, the multi-phase material with smooth transition between phases can be designed and produced. This is a concept of functionally graded materials (FGM).

An FGM is a composite material with the volume fractions of the constituents varying gradually in the designed profile. FGM is usually a mixture of ceramic and metal phases. The ceramic phase provides the high temperature resistance because of its low thermal conductivity, while metal phase prevents fracture caused by stress due to high temperature gradient. FGM provides opportunity to build a lightweight structure with unique properties that cannot be attained using a homogeneous material. However, the design of composition distribution within FGM for particular needs can be a challenging task.

The composition distribution within FGM can be designed in a systematic way by the optimization procedure [18]. The optimization method is strictly related to the area of applicability of FGM. The objective function depends on the problem considered and usually includes a measure of stress [3, 6], fracture resistance, temperature distribution [13, 18], strain energy and peak of effective stresses. As design parameters one can choose for instance thickness and the volume fraction of FGM interlayer's or parameters of thermal stress distribution. The review of optimization of FGM can be found in [2].

A separate class of optimization constitutes the topology optimization [1, 9]. The topology optimization can be viewed as a process of changing position of material interfaces in pseudo-time. The material interfaces are treated as the zero level set function [14, 15]. Evolution of this function will result in changing shape of the material interfaces. However, as known, the implementation may be problematic when to minimize the objective function one material should be created inside another one. To allow creation of one material inside another, the material topological derivative should be performed. Examples of topological optimization can be found in [4, 12, 19].

In order to produce an FGM structure which is resistant to thermo-mechanical loading, it is essential to determine the magnitude of thermal stresses and to design spatial distribution of the FGM phases. In this paper the robust optimization method of FGM is proposed for combined cyclic thermal and mechanical loadings. The design of the structure being under high cyclic thermal loading was possible after replacing this loading by its simplified representation. As a

theoretical background for finding the optimal distribution of materials in FGM we have selected multi-criterion optimization. The application to design of an exhaust valve of combustion engine is presented, see schematic representation of the axisymmetric valve model in Fig. 1.
In many engineering structures, thermal stresses are sufficiently large to generate cracks. Such a situation occurs in engine valves. Current valves are a result of many years of development, tests and checks. But necessity to reduce of energy consumption and needs of longer lifetime of mechanical parts implies application of new materials. FGM, as a composite of two or several materials, can solve many engineering problems. When one wants to join two or more materials together, the interface stresses usually occurs. FGM can significantly reduce stresses at interfaces of joined materials by connection with graded phase profile. Additionally, FGM can improve interface properties of samples by decreasing friction and wear. However, in case of engine valves, as shown by Szymczyk [17], thermal stresses at interfaces of FGM are very high. The valve with standard FGM coating will not survive under such conditions. We propose to solve a problem of joining two materials by applying a new technology of smooth evolution of volume fractions of two phases. Technologically it is not only possible but nowadays it is feasible. The problem remains how to design distribution of material phases. The present paper gives answer to this question. The ceramic-metal valve is optimized to gain its resistivity against cracking and assuming safety with respect to excessive plastic flow.

2 The proposed optimization method

The proposed methodology explores two parameters as a measure of tensile stress and effective plastic stress during process of transient thermal loading. The first is the maximum tensile stress σ_{cr} at a particular point and at a particular time instant and the second is the effective Mises stress σ_{ef}. Performing simulation of the whole process, we can extract maximum values of σ_{cr} and σ_{ef} during the process. As the scaling parameters the crack resistivity σ_{cr}^{lim} and yield resistivity σ_{ef}^{lim} at each of points are taken. Crack resistivity and yield resistivity depend on specific phase composition at the point and some rule of mixture is needed to specify their dependence on the volume fraction. The mean value of the Hashin-Shtrikman bounds [10] are taken for Young moduli and Poisson ratio (the randomly positioned particles are assumed). For all other material parameters like yield strength, thermal conductivity, thermal capacity, and thermal expansion coefficient, the simple Vegard's rule was used. Some notes are necessary about the tensile strength of composite material. Under monotonic loading, the tensile strength of composite with low ceramic content generally increases. But under cyclic loading mechanical behaviour of particle reinforced composites may be different. Mechanical properties of particle reinforced composites depend on size, shape, and spacing of precipitates [5]. Additionally, at high temperatures, the difference between thermal expansion coefficients of metal matrix and ceramic phase leads to a high concentration of stresses at inclusion interfaces. Those concentrations (depending on shape of inclusions), under high-cycle loading, generally lead to decrease of the tensile strength of composite. Therefore for safe design, the monotonic decrease of the tensile strength versus ceramic content is assumed.

Because the used small strain thermo-mechanical equations are standard, we do not duplicate them here. The proposed procedure can also be applied without modifications to finite strain formulation. The particular numerical implementation of axisymmetric valve model in examples shown in the next sections is as follows: 8-node serendipity element, the time step length is set as

$\triangle t = 1\, s$, the transient problem is integrated with the backward Euler method, the information about volume fraction of ceramic phase is updated at each Gauss point [11].
The optimization procedure starts from uniform distribution of ceramic phase. We want reduce concentration of the ceramic phase at places of high tensile stresses and increase the ceramic phase density at places of high effective stresses. A balance between those two sources leads to optimal, in the sense of the objective functional, distribution of ceramic phase. The optimization problem of FGM profile is formulated as follows: specify the field of distribution of ceramic phase volume fraction x within the metal matrix, such that the effect of maximal tensile and effective stresses are balanced. Such a balance is controlled through the weight factor β. The objective functional is proposed in the form:

$$J_{obj} = \left[\frac{\sigma_{ef}}{\sigma_{ef}^{lim}} + \beta \, \frac{\sigma_{cr}}{\sigma_{cr}^{lim}} \right], \tag{1}$$

where the crack resistivity σ_{cr}^{lim} and the yield resistivity σ_{ef}^{lim} depend on their initial values $\sigma_{cr\,0}^{lim}$, $\sigma_{ef\,0}^{lim}$ and on the specific phase composition x:

$$\sigma_{ef}^{lim} = \sigma_{ef\,0}^{lim} + A\, x\, \sigma_{ef\,0}^{lim}, \tag{2}$$

$$\sigma_{cr}^{lim} = \sigma_{cr\,0}^{lim} - B\, x\, \sigma_{cr\,0}^{lim}. \tag{3}$$

The variation of the objective functional (1) with respect to volumetric ceramic phase fraction x takes the form

$$\delta J_{obj} = - \left(\frac{\sigma_{ef}}{\sigma_{ef}^{lim\,2}} \, \delta \sigma_{ef}^{lim} + \beta \frac{\sigma_{cr}}{\sigma_{cr}^{lim\,2}} \, \delta \sigma_{cr}^{lim} \right) + \left(\frac{1}{\sigma_{ef}^{lim}} \, \delta \sigma_{ef} + \beta \frac{1}{\sigma_{cr}^{lim}} \, \delta \sigma_{cr} \right). \tag{4}$$

Because stress field usually varies during the transition process, we neglect in (4) the terms with implicit variations of σ_{ef} and σ_{cr} and consider only the explicit terms of sensitivity

$$\delta J_{obj} = - \left(\frac{\sigma_{ef}\, \sigma_{ef\,0}^{lim}}{\sigma_{ef}^{lim\,2}} \, A - \beta \frac{\sigma_{cr}\, \sigma_{cr\,0}^{lim}}{\sigma_{cr}^{lim\,2}} \, B \right) \delta x = - \left(J_{pl} - \beta J_{cr} \right) \, \delta x, \tag{5}$$

with non-dimensional measures of tensile and effective stresses relative to their critical values

$$J_{pl} = A \, \frac{\sigma_{ef}\, \sigma_{ef\,0}^{lim}}{\sigma_{ef}^{lim\,2}}, \tag{6}$$

$$J_{cr} = B \, \frac{\sigma_{cr}\, \sigma_{cr\,0}^{lim}}{\sigma_{cr}^{lim\,2}}. \tag{7}$$

The optimality condition is fulfilled when $\delta J_{obj} = 0$ i.e. when $J_{pl} = \beta J_{cr}$, see Eq. (5). The complete formulation containing both explicit and implicit sensitivity terms will be discussed in the separate paper by following the sensitivity analysis presented in [7, 8]. The optimization method used is of heuristic nature and optimality cannot be generally guaranteed. Such proof of optimal design is probably impossible, due to nonlinearity of the analysed processes and properties of materials. But even the proposed method violates a strict mathematical proof of optimality, it allows to speed up design of highly complicated physical process. Therefore, the proposed method may be viewed as a practical design method.

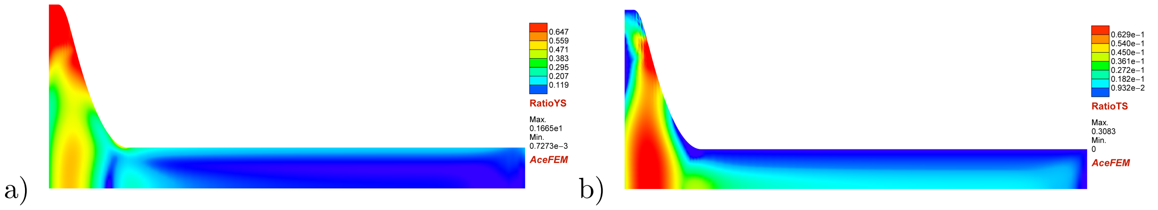


Figure 2: Analysis of ceramic exhaust valve with initial, homogeneous distribution of ceramic phase Al_2O_3 within $NiAl$ matrix ($x_{ini} = 0.0$); a) and b) distribution of yield strength and crack strength parameters J_{pl} and J_{cr}, defined by Eqs (6) and (7) respectively at time $t = 2$ s of the process.

3 Optimization procedure

The optimization procedure starts from the uniform ceramic distribution of Al_2O_3 within the metal matrix of $NiAl$. We have performed optimizations with assumed minimal volume fraction (0%) or with maximal volume fraction (30%) at the beginning of optimization. The iterative design is performed through the following procedure

1. Initial state – uniform ceramic phase distribution.

2. Perform simulation of thermal transient process (for time period $t_0 - t_{max}$).
   For each point of the body determine the maximal effective stress ratio σ_{ef} and maximal tensile stress ratio σ_{cr} during the transient process.

$$\sigma_{ef}^{max} = \max_t \left(\frac{\sigma_{ef}}{\sigma_{ef}^{lim}} \right), \tag{8}$$

$$\sigma_{cr}^{max} = \max_t \left(\frac{\sigma_{cr}}{\sigma_{cr}^{lim}} \right). \tag{9}$$

   Here σ_{ef}^{lim} and σ_{cr}^{lim} are the limit stress values at a particular point at the time when the maximal effective and the maximal tensile stresses have been attained, respectively.

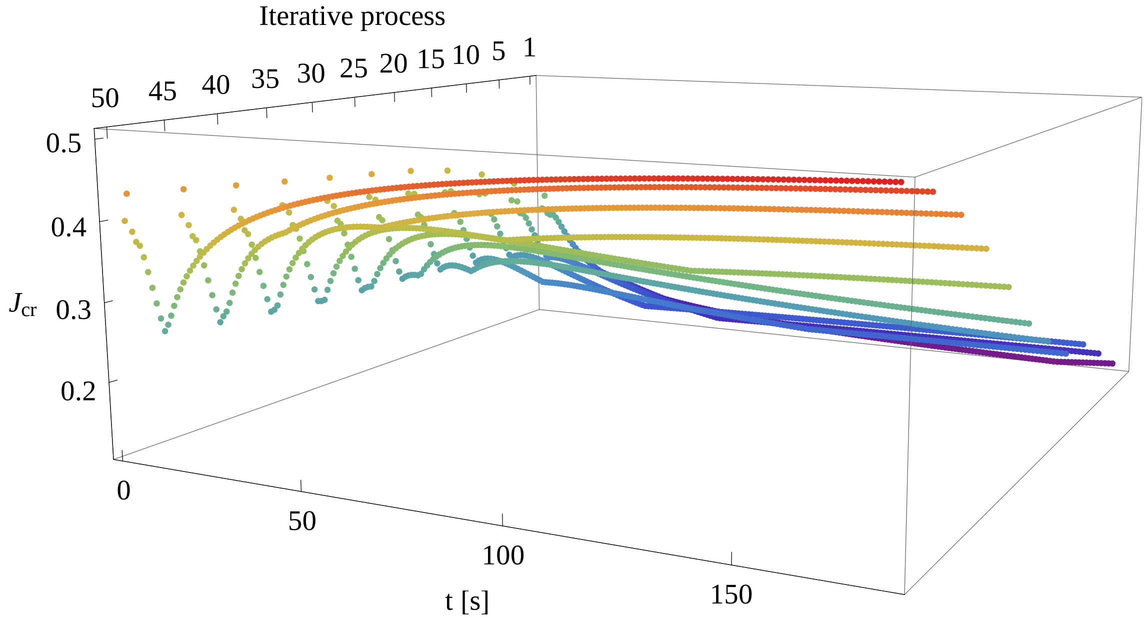
3. Then, from Eqs (6) and (7) calculate derivative of the objective functional (5), with replaced values of stresses by theirs maximal values during the process, see Eqs (8,9). The rations σ_{ef}^{max} and σ_{cr}^{max} should be less than one in order to assure that the structure does not change its geometry and quality as an effect of excessive plastic flow or generation of cracks.

4. Redesign the ceramic content proceeds at each point according to the following equation:

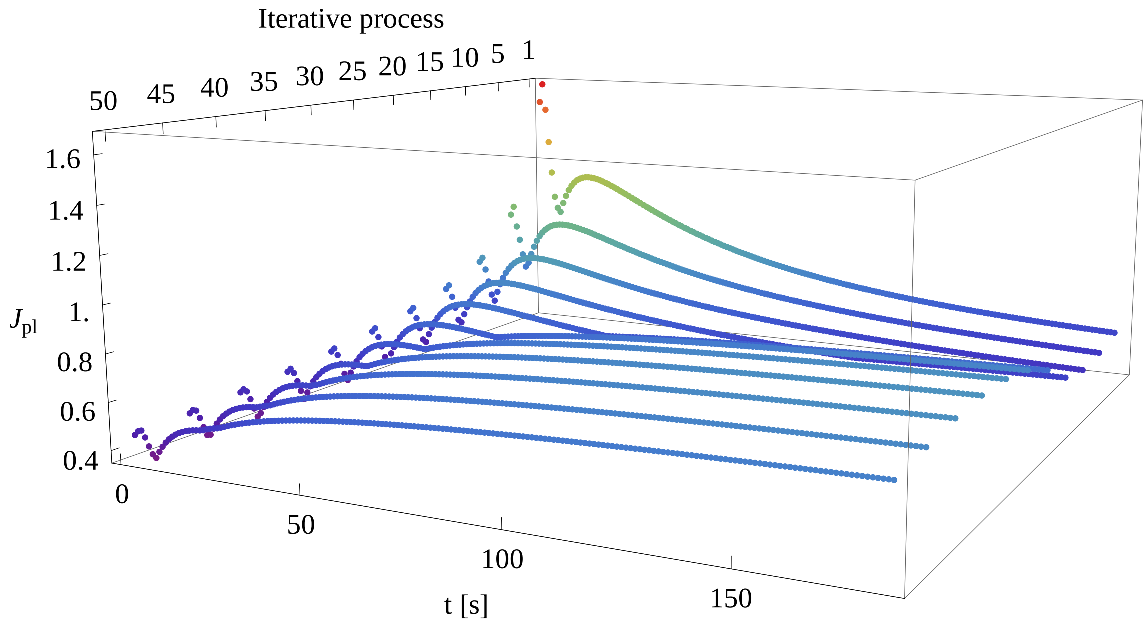
$$\frac{\Delta x}{x_{max}} = -\lambda\, \delta J_{obj} = \lambda\, (J_{pl} - \beta J_{cr}), \tag{10}$$

   where λ is the proportionality parameter depending on particular problem considered. and limit value of ceramic phase density x_{max} respectively. Additionally, an obvious constraint $0 \leq x \leq x_{max}$ should be fulfilled.

5. Repeat steps (2)–(4) until some global condition is fulfilled e.g. $|\delta J_{obj}| < 0.05$ or $\delta J_{obj} > 0$.



a)



b)

Figure 3: Iterative process of rebuilding ceramic volume fraction; a) and b) show evolution of crack strength parameter J_{cr} and yield strength parameter J_{pl} respectively, see Eqs. (7) and (6). Thermomechanical loading (combustion process) starts at $t = 0$. There are 50 transient thermo-mechanical processes, each one for different ceramic phase distribution.

By applying the above iteration procedure, an optimal distribution of ceramic phase can be found. Because stress distribution is continuous, the obtained FGM has also continuous distribution of ceramic phase. Thus, the proposed method shares merits of standard shape optimization and topology optimization because it allows for creation of one phase of material inside another. The following numerical example shows practical usefulness of the method.

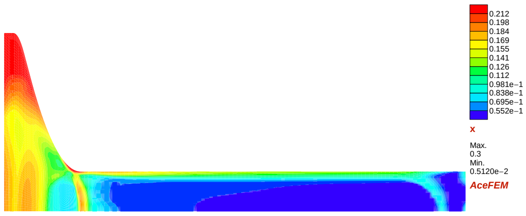


Figure 4: Ceramic exhaust valve analysis with optimal (for $\beta = 1.0$ in Eq. (1)), inhomogeneous distribution of ceramic phase.

4 Example of an engine valve optimization

Let us consider an engine exhaust valve schematically illustrated in Fig. 1. The valve is subjected to mechanical loading, marked by blue colour, and to thermal transient loading, marked by red colour. The numerical analysis of valve, cf. [17], shows that at the interface between ceramic coating and the metal substrate, a very high stresses are observed. Additionally, when valve is subjected to cyclic thermal loading, as presented in [16], the numerical optimization becomes very complex. Without simplification of the model, the optimization would be very time consuming. The simplification of boundary conditions is proposed in order to account for physical aspects of analysed process and to allow for optimization procedure.

High-cycle thermal and mechanical loading - simplification The simplification of boundary conditions is performed by replacing the true heat loading by its averaged values over the one cycle of engine operation, while the mechanical loading condition corresponds to maximum loading during one cycle. Thus, the high cyclic thermal and mechanical loadings are replaced by equivalent heat flow conditions and the most unfavourable static loading.

The heat transfer between the valve and surroundings is described by the standard equation $q = TCC(T_s - T_v)$, where TCC, T_s, and T_v denote the thermal contact coefficient, temperature of the surrounded medium and temperature of the valve on the particular surface. The thermal contact coefficient (in $W/m^2\,°\mathrm{C}$) between the valve, see description in Fig. 1, and gases at cylinder (a), valve seat (b), exhaust port (c), valve guide (d) are assumed equal to 850 ($T_s = 900\,°\mathrm{C}$), 3000 ($T_s = 500\,°\mathrm{C}$), 500 ($T_s = 500\,°\mathrm{C}$), 2000 ($T_s = 400\,°\mathrm{C}$), respectively. The values of TCC and temperature are based on data from [16, 20] and from unpublished sources. The gas pressure is equal to 60 kPa. The transient analysis of stress and temperature fields in the analysed valve (subjected to the above simplified thermal and mechanical loadings) is performed in the design study.

The optimization of ceramic phase distribution The valve returns generated heat to the remaining portion of an engine through the contact surface b or to the air through surfaces c and d. Initially the valve is cold and when the engine starts, a very high heat flux from the combustion engine acts on the valve. The temperature of the valve head rapidly increases, while the rest of the valve is still cold. The main source of stress results from non-uniform temperature distribution and its maximum occurs at the initial instant of engine work. This temperature inhomogeneity can lead to high thermal stresses inducing cracking and plastic flow. In order to avoid cracking and to minimize plastic deformation, the optimization of ceramic phase distribution is performed with procedure proposed in the previous section. For the considered valve

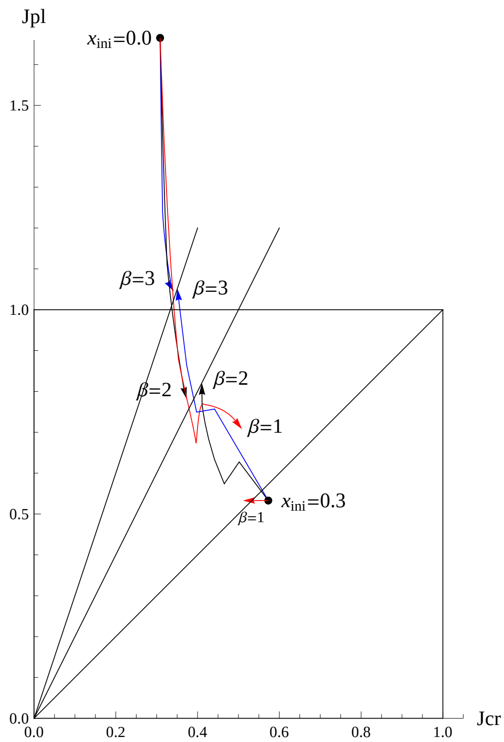


Figure 5: Paths of optimization processes with the parameter β in Eq. (1) equals one, two, and three. Optimizations start from the state of homogeneous density of ceramic phase equal to $x_{ini} = 0.0$ or $x_{ini} = 0.3$.

case, we assumed parameters $\beta = 1.0$, see Eq. (1). The value of parameter λ in Eq. (10) depends on the iterative process and needs to be adjusted through trials and tests. If λ is too high some spurious modes can occur. Because the solution of the proposed algorithm depends on the step length, λ should be as low as possible. The ending condition of optimization process is not applied in order to see a wide range of system evolution.

Fig. 2 shows simulation results for process with homogeneous distribution of ceramic phase. The maximal values of crack and yield strength parameters are observed at the time $t = 2\,s$ of the process, cf. Fig. 2a and Fig. 2b respectively. The optimization iterations are visualized in Fig. 3, where the evolutions of J_{cr} and J_{pl} during transient thermal loading processes with different ceramic phase distributions are shown. After 40 iterations, the final distribution of Al_2O_3 is attained as presented in Fig. 4. Additional iterations after 40 steps of optimization did not change the ceramic phase distribution. Thus, one can observe that the final stage of optimization could be attained through stopping condition like for instance $\delta J_{obj} < \delta J_{obj}^{crit}$, where δJ_{obj}^{crit} is some critical value. We have performed several simulations with different form of the objective functional. The parameter β in Eq. (1) was assumed to be equal one, two, and three. Additionally, the optimization procedures started from homogeneous density of ceramic phase equal to $x_{ini} = 0.0$ or $x_{ini} = 0.3$. The results of optimizations are summarized in Fig. 5, where paths of optimization processes were plotted. The different optimization functionals (corresponding to different values of the weight factor β) lead to different optimal distributions of the ceramic phases.

5 Summary and conclusions

The robust optimization method of FGM under combined cyclic thermal and mechanical loading is proposed. The proposed methodology can be especially useful in the design procedure of elements with complex shapes and under complex transient loading conditions.

The presented numerical example illustrates the optimal volume fraction distribution of the ceramic phase Al_2O_3 within the metal matrix of $NiAl$ for mechanical and thermal constraints. The analysis of FGM engine valves was significantly simplified to allow for optimization of lightweight valves. The method proposed permits manufacturing of products with improved surface properties (low-wear surface) and with reduced weight. It is worth to note that making valves with standard ceramic coating leads to very high values of thermal stresses because of the difference between thermal expansion coefficients of ceramic coating and bulk material. The current manufacturing technologies allow to produce designed reinforced metal matrix $NiAl$ with ceramic phase of Al_2O_3. Thus, the proposed method can be useful for practical design of thermal resistant structures.

The objective functional used, see Eqs. (1),(6), and (7), represents the sensitivity of structure on incidentally applied high stresses. Other measures, like for instance the integrated measures over time period of engine operation $J_{cr}^t = \int J_{cr}\,dt$ and $J_{pl}^t = \int J_{pl}\,dt$ could provide the global assessment of safety of valve relative to fatigue failure. Such modifications allow for flexible adjustment of the objective functional to the particular needs. One of the most valuable properties of the proposed method is that there is no need to a priori specify an FGM variation function.

Acknowledgements

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