Two-dimensional Thermomechanical Analysis and Optimization of Functionally Graded Materials

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Summary

In this paper, we study the two-dimensional volume fraction optimization of heat resisting metal/ceramic functionally graded materials (FGMs). The plane stress static thermoelastic behavior of a FGM is analyzed using the element-free Galerkin method. The effective material properties of the two-phase FGM is estimated using the Mori-Tanaka and self consistent schemes. A genetic algorithm optimization procedure is used to determine the ceramic volume fraction distribution that would minimize the peak effective stress.

Introduction

Advanced composite materials offer numerous superior properties to metallic materials, like high specific strength and high specific stiffness. For example, a layer of a ceramic material can be bonded to the surface of a metallic structure to form a thermal barrier coating in high-temperature applications. However, the abrupt transition in material properties across the interface between discrete materials can result in large interlaminar stresses, and eventually delamination failure. One way to overcome these adverse effects is to use functionally graded materials. FGMs are inhomogeneous materials, consisting of two (or more) different materials, engineered to have a continuously varying spatial composition profile. The choice of material phases is motivated by functional performance requirements. The determination of the optimal volume fraction distributions of the constituents is critical in the design of FGMs. Here we analyze the thermal stress in FGMs using the element-free Galerkin method [1] and optimize the volume fraction distribution using genetic algorithms [2]. The volume fraction at a point is obtained from nodal volume fraction parameters using piecewise bicubic interpolation. Numerical results are presented for a Ni-Al_2O_3 FGM that is subjected to a uniform temperature change. It shows that the proposed approach can lead to better designs for FGMs than conventional gradient based optimization methods.

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Thermoelasticity Equations

We consider the infinitesimal static thermoelastic deformations of an isotropic body which occupies a domain Ω. The rectangular Cartesian coordinates x_i are used to describe its deformation in the unstressed reference state. The mechanical equilibrium and constitutive equations for an isotropic material are

$$\operatorname{div}\sigma + \rho\mathbf{b} = \mathbf{0}, \quad \sigma = \lambda(\operatorname{tr}\varepsilon)\mathbf{1} + 2\mu\varepsilon - \beta\theta\mathbf{1}, \tag{1}$$

where σ is the Cauchy stress tensor, $\mathbf{b}$ is the body force per unit mass, ρ is the mass density, ε is the infinitesimal strain tensor, $\mathbf{1}$ the identity tensor, λ and μ are the Lamé constants, θ is the change in temperature from the reference state and β the stress-temperature modulus. The infinitesimal strain tensor is related to the displacement vector $\mathbf{u}$ by $\varepsilon = (\nabla\mathbf{u} + \nabla^T\mathbf{u})/\mathbf{2}$.

At every point $\mathbf{x}$ on the boundary Γ, either the displacement component $u_i = \hat{u}_i$ or the mechanical traction $\sigma_{ij}n_j = \hat{\sigma}_i$ is prescribed in each coordinate direction x_i, which can be stated as

$$\mathbf{S}\mathbf{u} + (\mathbf{1} - \mathbf{S})\sigma\,\mathbf{n} = \mathbf{S}\hat{\mathbf{u}} + (\mathbf{1} - \mathbf{S})\hat{\sigma} \quad \text{on} \quad \Gamma, \tag{2}$$

where $\mathbf{S}$ is a diagonal matrix with either 0 or 1 on the diagonals.

Element-free Galerkin Method

Let ξ be a smooth vector test function such that $\mathbf{S}\xi = \mathbf{0}$ on Γ. Taking the dot product of $(1)_1$ with ξ and integrating over the domain, and utilizing the Duhamel-Nuemann thermoelastic-elastic correspondence principle results in the weak formulation

$$\int_\Omega \sigma : \varepsilon(\xi)\, d\Omega + \delta \int_\Gamma \mathbf{S}\mathbf{u}\cdot\xi\, d\Gamma = \int_\Omega \rho\mathbf{b}\cdot\xi\, d\Omega + \int_\Gamma (\mathbf{1} - \mathbf{S})\hat{\sigma}\cdot\xi\, d\Gamma - \int_\Gamma \beta\theta\mathbf{S}\mathbf{n}\cdot\xi\, d\Gamma + \int_\Omega \beta\theta\operatorname{div}\xi\, d\Omega + \delta\int_\Gamma \mathbf{S}\hat{\mathbf{u}}\cdot\xi\, d\Gamma, \tag{3}$$

where δ is the mechanical penalty parameter, which is chosen to be in the range 10^3 to 10^7 times the Young's modulus. We select the following discretization of the scalar temperature field at a position $\mathbf{x}$ in the domain:

$$u_i = \phi_k(\mathbf{x})\bar{u}_{ki}, \quad k = 1, 2, ..., N;\ i = 1, 2, \tag{4}$$

where N is the number of nodes in the domain, $\phi_k(\mathbf{x})$ are the MLS approximation functions [1] and $\bar{u}_{ki}$ are the nodal displacement parameters which are to be solved for. In the Galerkin formulation, the test functions are also discretized as

$$\xi_i = \phi_k(\mathbf{x})\bar{\xi}_{ki}. \tag{5}$$

Substitution of (4) and (5) into the weak formulation (3) yields the following system of algebraic equations for the nodal displacement parameters,

$$\mathbf{L}_{jk}\,\bar{\mathbf{u}}_k = \mathbf{f}_j, \quad k,j = 1,2,...,N, \tag{6}$$

where the matrices in (6) are defined as

$$\mathbf{L}_{jk} = \int_\Omega \mathbf{D}_j^T\mathbf{C}\mathbf{D}_k\,d\Omega + \delta\int_\Gamma \mathbf{\Phi}_j\mathbf{S}\mathbf{\Phi}_k\,d\Gamma,$$

$$\mathbf{f}_j = \int_\Omega \rho\mathbf{\Phi}_j\mathbf{b}\,d\Omega + \int_\Gamma \mathbf{\Phi}_j(\mathbf{I}-\mathbf{S})\hat{\sigma}\,d\Gamma + \int_\Omega \beta\theta\mathbf{\Psi}_j\,d\Omega$$
$$- \int_\Gamma \beta\theta\mathbf{\Phi}_j\mathbf{S}\mathbf{n}\,d\Gamma + \delta\int_\Gamma \mathbf{\Phi}_j\mathbf{S}\hat{\mathbf{u}}\,d\Gamma,$$

$$\mathbf{\Phi}_j = \begin{bmatrix} \phi_j & 0 \\ 0 & \phi_j \end{bmatrix},\ \mathbf{D}_j = \begin{bmatrix} \phi_{j,1} & 0 \\ 0 & \phi_{j,2} \\ \phi_{j,2} & \phi_{j,1} \end{bmatrix},\ \bar{\mathbf{u}}_k = \begin{Bmatrix} \bar{u}_{k1} \\ \bar{u}_{k2} \end{Bmatrix},$$

$$\mathbf{\Psi}_j = \begin{Bmatrix} \phi_{j,1} \\ \phi_{j,2} \end{Bmatrix}, \mathbf{C} = \frac{E}{1-\nu^2}\begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & (1-\nu)/2 \end{bmatrix},\ \beta = \frac{\alpha E}{1-\nu}.$$

Volume Fraction Interpolation Scheme

The volume fractions are chosen over a regularly spaced rectangular grid. Between the grid points, the volume fraction is obtained using piecewise bicubic interpolation. The restriction of the volume fraction to remain between the physically valid bounds of 0 and 1 is achieved by setting allowable limits on the partial derivatives used in the bicubic interpolation [3]. The volume fraction $V(x,y)$ over a rectangular grid element of the domain is interpolated from the nodal volume fractions $V(x_i,y_j)$ and the partial derivatives $V_x(x_i,y_j)$, $V_y(x_i,y_j)$ and $V_{xy}(x_i,y_j)$ at the grid nodes using Hermite basis functions. The partial derivatives of the volume fraction distribution profile at a node (x_i,y_j) are estimated using three point difference estimates, which are then projected onto the valid range.

Genetic Algorithm Optimization

An important limitation of traditional classical optimization methods, such as the gradient-based methods, is that they tend to get stuck at a suboptimal solution. Genetic algorithms (GA) are better at finding global solutions and they are easy to parallelize. A GA is a search and optimization method that mimics the evolutionary principles and chromosomal processing in natural genetics [2]. A GA begins its search with a random population of design parameters (genes), usually coded in binary string structures (chromosome). In the present case, each volume fraction parameter at the grid points corresponds to a gene that describes the design. The population of solutions is modified to a new population by applying three operators similar to natural genetic operators - reproduction, crossover, and mutation. The algorithm systematically analyzes each individual of the population of designs according to set specifications (geometry, boundary conditions and thermomechanical loads) and assigns it a fitness rating which reflects the designer's goals. This fitness rating is then used to determine which designs perform better than others, thereby enabling the genetic algorithm to determine the designs that are weak and must be eliminated (survival of the fittest), thus producing the next generation of designs. The process is iterated over many generations until the optimal design is identified. Since the optimization parameters, namely the volume fraction parameters, are real valued and continuous, we have implemented a real-coded GA. Unlike a binary-coded GA, the crossover and mutation operators act directly upon the real chromosome parameters, not on a binary coded version of the parameters, which allows the GA to operate in a continuous search space. Several different real-coded GA recombination operators have been developed, including the unimodal normal distribution crossover (UNDX) operator and simulated binary crossover (SBX) operator [4]. We have utilized the simulated binary operator and a tournament selection process in the reproduction phase of the GA.

Results and Discussion

Consider the model problem depicted in Fig. 1 which consists of a half of a simply supported three-layered Ni-Al_2O_3 heat-resisting FGM that is uniformly cooled down to 300 K from uniform initial temperature of 1000 K [5]. The goal is to optimally tailor the volume fraction distribution in the design region to minimize the effective stress. Cho and Ha [5] used

finite element simulations, piecewise bilinear approximations for the volume fractions and a gradient based optimization algorithm to decrease the peak effective stress to 268 MPa for this configuration.

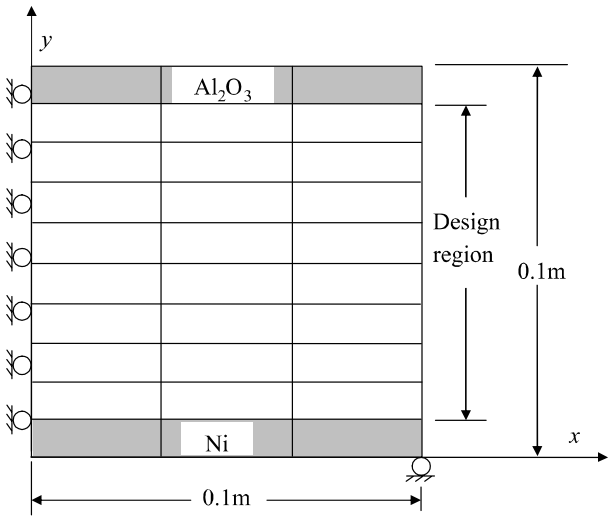

Figure 1: Simply supported FGM subjected to uniform temperature change

We have analyzed the same problem using the element-free Galerkin method and optimized the volume fraction distribution using a real-coded GA. The EFG analysis is performed with 144 regularly spaced nodes and the mechanical penalty parameter $\delta = 7 \times 10^{15}$. A total of 28 volume fraction parameters at regularly spaced nodes is used to optimize the volume fraction distribution in the design region. The effective material properties at a point are estimated using either the Mori-Tanaka scheme or the self-consistent scheme, depending on the local ceramic volume fraction as described by Vel and Batra [6]. The population size of the GA is 280 and the optimization is terminated at 152 generations after the effective stress converged to its minimum value. Figure 2(b) shows the effective stress distribution corresponding to a linear grading of the volume fraction depicted in Fig. 2(a). The peak effective stress of 254 MPa occurs at the top surface of the plate. The optimized volume fraction distribution is depicted in Fig. 2(c). The peak effective stress corresponding to the optimized material distribution is 135 MPa (Fig. 2d), which represents a significant reduction. The results show that the proposed approach using the element-free Galerkin method and genetic algorithms can lead to better designs for FGMs than conventional gradient based optimization methods.

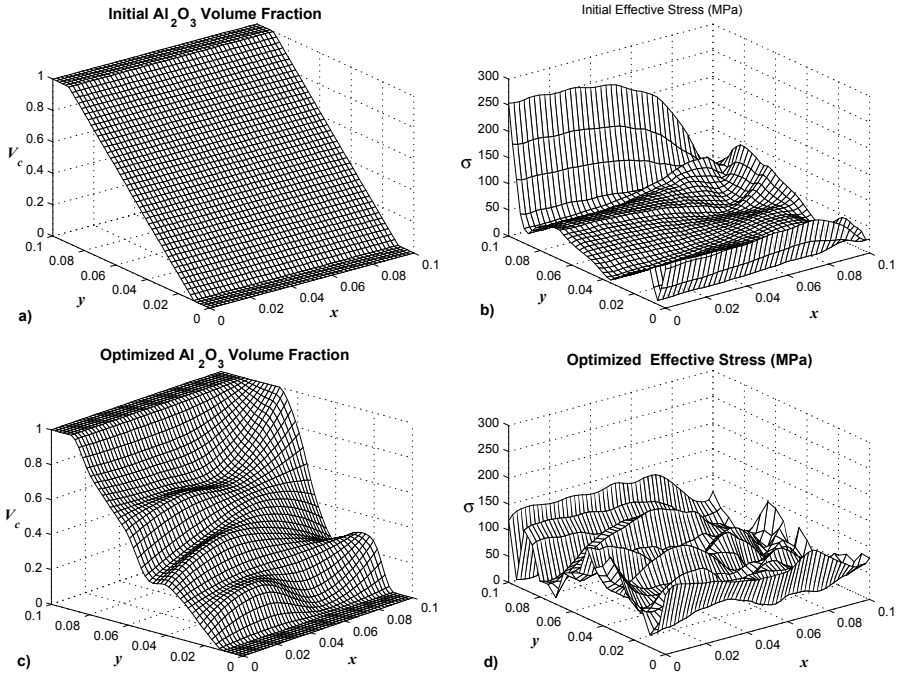

Figure 2: a) initial ceramic volume fraction, b) initial effective stress, c) optimized ceramic volume fraction and d) optimized effective stress.

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