Application of the Micromechanical Models for Estimation of the Optimal Design of Metal-Ceramic composites

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Abstract

Metal-ceramic composites produced by melt infiltration of the ceramic preform were studied. The ceramic preform of the studied materials is manufactured through freeze-casting process. The microstructure of these materials can be presented as distribution of the lamellar domains. Micromechanical models were used for the calculation of the effective elastic properties of the domains. The minimum compliance problem was solved for sample subjected to the four-point and three-point bending tests. The optimal orientation and volume fracture of the micro constituents were identified using different element models. The difference between the initial and optimized design was analyzed. The convergence of the provided optimization procedure was very rapid.

Keywords: metal-ceramic composites, micromechanical modeling, minimum compliance

1. Introduction

The development of materials with prescribed material properties or optimal microstructure for particular loading cases is very interesting from the view of future industrial applications. Innovative metal-ceramic composites (MCCs) produced via melt-infiltration of freeze-casting ceramic preform [1] show microstructure with lamellar domains [2]. The geometrical characteristics of the domains are dependent on the manufacturing parameters. FE-calculations and micromechanical modeling were proposed in [3] for determination of the effective elastic properties of the single domains. The results of the both procedures are close to each other and show good correspondence to the experimentally obtained elastic properties.

Once implemented, the micromechanical model is fast in calculating the elastic properties and by simple change of the parameters (volume fraction, orientation etc.) of the domain the effective properties of the microstructure with new geometry can be calculated. It can be easily incorporated in other model calculations such as microstructure optimization, which needs fast estimates of the effective properties of variable microstructures. In this publication we have applied a micromechanical model for elements for micromechanical modeling of MCCs. The microstructure optimization was provided using the methodology proposed in [4, 5].

Figure 1: Typical microstructure of the studied material (light gray is ceramic and dark grey is the metal alloy) and one domain with orientation $\alpha$ to the global coordinate system.

2. Studied materials

The typical microstructure of the studied material is presented in Figure 1 and consists of two micro constituents: ceramic inclusions (Al2O3, light gray) and a metal matrix (Al–Si-alloy, dark gray). The ceramic preform of the studied materials is produced through freeze-casting and its architecture is induced through the geometry of the growing ice crystals and is constant in this direction. The composites were produced using melt infiltration of these
ceramic performs and can be adequately modeled in 2D [2]. Ceramic inclusions are lamellar and form domains with the same orientation of lamella (see Figure 1). Both micro constituents are isotropic and have large contrast in elastic modulus: \( E_c = 400 \text{GPa} \) (for ceramic) and \( E_m = 77.6 \text{GPa} \) (for metal). The Poisson values for both materials are close to each other: \( \nu_c = 0.25 \) and \( \nu_m = 0.3 \). The difference in elastic modulus significantly influences the stiffness of the resulting composite and depends on the volume fractions of the micro constituents.

In our case the inclusions can be approximated by parallel elliptical cylinders with the same ellipse-axis ratios. The typical half-axis ratio for this material was determined in [3] and it lies between 0.1 and 0.6.

3. Micromechanical modeling of the single domain

Different homogenization methods can be used for the calculation of the effective elastic properties of the single domain.

In this paper we present two of them: The first one was used for the homogenization of the laminate material in [4] and the second one is the Mori-Tanka model, which was used for the homogenization of the studied material in [3]. For the first homogenization procedure it is supposed that the single domain can be approximated as laminate and for the homogenization procedure the formulae can be used [4]:

\[
\begin{align*}
\tilde{C}_{1111} &= M(C_{1111}) - M\left(\frac{C_{1222}^2}{C_{2222}}\right) + M\left(\frac{C_{1122}^2}{C_{2222}}\right) - M\left(\frac{1}{C_{2222}}\right)^{-1}, \\
\tilde{C}_{2222} &= M\left(\frac{1}{C_{2222}}\right)^{-1}, \\
\tilde{C}_{1122} &= M\left(\frac{C_{1122}}{C_{2222}}\right) M\left(\frac{1}{C_{2222}}\right)^{-1}, \\
\tilde{C}_{1212} &= M\left(\frac{1}{C_{1212}}\right)^{-1},
\end{align*}
\]  

where the average function \( M(C_{ijkl}) = f_c C_{ijkl}^c + (1 - f_c) C_{ijkl}^m \) and direction 1 is the layer direction.

The approximation of the effective elastic properties of the domain using the Mori-Tanaka model has the following form:

\[
\tilde{C} = C^c + (1 - f_c)(C^m - C^c) : A_{(MT)}^m,
\]

\[
A_{(MT)}^m = [I^4 + f_c S_c : (C^c)^{-1} : (C^m - C^c)]^{-1},
\]

where \( I^4 \) is the symmetric fourth-order unit tensor; \( C^c, C^m \) are the stiffness tensors of the ceramic and metal phases; \( f_c \) is the volume fraction of the ceramic phase in the domain. In this model it is supposed, that the inclusions are approximated as ellipses and the components of the Eshelby tensor \( S_c \) can be presented as functions of the half-axes of the ellipses and the Poisson ratio of the matrix [6].

The inverse Mori-Tanka model [3] can be also used for alternative calculations of the elastic properties of the domain.

4. Microstructure optimization

4.1. Problem formulation

Microstructure optimization of a MCC will be provided using the FE-method. Each element presents a single domain with particular orientation and volume fraction of the ceramics. The optimal design problem in this formulation is to find the optimal choice of the stiffness tensor in each element \( C_{ijkl}(x) \), \( x \in \Omega \subset \mathbb{R}^2 \) that depends on two design variables: the ceramic content \( f_c \) and domain orientation \( \alpha \).

Introduce the energy bilinear form \( a(u, v) \) and the load linear form \( l(v) \):
\[ a(u, v) = \int_{\Omega} C_{ijkl}(x) \varepsilon_{ij}(u) \varepsilon_{kl}(v) \, d\Omega, \quad (3) \]

\[ l(v) = \int_{\Omega} f \, v \, d\Omega + \int_{\Gamma_T} t \, v \, ds, \]

With the linearized strain \( \varepsilon_{ij} \), the body forces \( f \) and the boundary tractions \( t \) on the traction part \( \Gamma_T \subset \Gamma \equiv \partial \Omega \) of the boundary. The minimum compliance (maximum global stiffness) problem has the form [4]

\[ \min_{u \in U, f_c, \alpha} \ l(u) \quad (4) \]

s.t.: \( a_c(u, v) = l(v), \quad \forall v \in U, \]

\[ C_{ijkl}(x) = \tilde{C}_{ijkl}(f_c(x), \alpha(x)), \]

\[ \int_{\Omega} f_c(x) \, d\Omega \leq F_c; \quad f_c \leq f_c(x) \leq f_c \max, \ x \in \Omega. \]

Here \( U \) is the space of kinematically admissible displacement fields; \( \tilde{C}_{ijkl} \) are the components of the effective stiffness tensor, which are calculated numerically using the homogenization procedure (see previous section, formulae (1)-(2)); \( F_c \) is the given amount of ceramic in \( \Omega \); \( f_c \min, f_c \max \in (0, 1) \) are the limits on the ceramic content in element.

4.2 Solution procedure

![Figure 2: Calculation flow for the optimization problem with two design variables.](image)

The used flow of computations is presented in Figure 2. The methodology proposed in [4, 5] was used for solving the optimization problem. The change of the strain energy with updating of the design variables for each iteration is shown in Figure 3 for four-point bending test (The iterative procedure consists of updating of two design variables: the ceramic content and the domain orientation proposed in [4, 5].)

![Figure 3: Changing in strain energy of the sample (four-point bending test) during updating of the design variables.](image)
Figure 4: Microstructure optimization of MCC (four-point bending test) using Mori-Tanaka model for calculation of the effective properties of the elements: a) FE-calculated distribution of the domain orientations (lines inside of the elements) and volume fraction of the ceramics (in grey scale) for the four-point bending test; b) stresses; c) strains distribution in optimal microstructure; d) strains distribution in initial microstructure with constant volume fraction of the ceramics $F_c=0.5$ and orientation angle $\alpha = 0$.

5. Numerical examples

The proposed methodology was applied for microstructure optimization of the MCC sample loaded by the three and four-point bending tests. The orientation of the element is characterized through the inclusions orientation $\alpha$. Using the algorithm proposed in the previous section the optimal microstructure was calculated. The design variables satisfy the following restrictions:

The volume fraction of the ceramic $F_c$ in the whole composite is equal to 0.5; $0.3 \leq f_c(x) \leq 0.6$ for the volume fraction of the ceramic in the domain and $\frac{\pi}{2} < \alpha < \frac{3\pi}{2}$ for the domain orientation.

Only in the first iteration the significant changes of the strain energy are visible. Optimal material design is presented in Figure 4a for four-point bending test and in Figure 5a for three-point bending test. The lines inside elements show the optimal orientation and the color of the element indicates the volume fraction of the ceramics.

In the optimal microstructure the domains, which are stiffer in lamella direction, are oriented along the direction of the major principle stress (see Figure 4 b and 5 b) and they have the maximal volume fraction of the ceramics.
Figure 5: Microstructure optimization of MCC (three-point bending test) using Mori-Tanaka model for calculation of the effective properties of the elements: a) FE-calculated distribution of the domain orientations (lines inside of the elements) and volume fraction of the ceramics (in grey scale) for the three-point bending test; b) stresses; c) strains distribution in optimal microstructure; d) strains distribution in initial microstructure with constant volume fraction of the ceramics $F_c=0.5$ and orientation angle $\alpha=0$.

Figures 4 c and 4 d (Figures 5c and 5d) show strains distributions in the optimal and initial microstructures and indicate changes induced through the optimization procedure.

Figure 6: Difference in optimal microstructure (four-point bending test) calculated using Laminate Model (1) and Mori-Tanaka Model (2) for calculation of the effective properties of the elements: a) Difference in ceramics content; b) Difference in orientation of the domains.
For better understanding of the influence of chosen homogenization procedure (chapter 3) on the result of the microstructure optimization the difference between results obtained using different methods for four-point bending test were calculated (see Figure 6). These differences are not significant with the exceptions of the regions along which the elements change orientation. In these regions some elements with effective properties calculated using different homogenization procedures can switch their orientation and ceramic content.

6. Conclusions
The main results obtained in provided studies are the following:
- A methodology for combination of the micromechanical models and the microstructure optimization problem for metal-ceramic composites are proposed.
- The minimum compliance problem was solved for the four-point and three-point bending tests. The optimal distribution of the ceramic and lamella orientation for each domain (element) was determined.
- The comparison of the strains distribution in the optimal and initial microstructures shows reduction of the strains in the optimal one. The reduction of the difference between the maximal and minimal strains $\varepsilon_{22}$ and $\varepsilon_{12}$ for optimal microstructure was found to be significant.
- The difference between optimal microstructures obtained using different homogenization procedures is not very significant with the exception of some elements lying in regions with rapid changes of the elements orientation.

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