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MULTI-OBJECTIVE OPTIMIZATION OF EFFECTIVE THERMO-MECHANICAL PROPERTIES OF METAL-CERAMIC COMPOSITES

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Abstract. *Micromechanical modelling of metal-ceramic composites has been carried out to obtain a material of required thermo-mechanical properties. Quantitative transition from phase properties and morphology to macroscopic properties of a composite has been modelled by mean-field approaches, including the self-consistent scheme. An optimization method has been developed for the objective function that expresses a distance between the required values of macro-variables and those determined for a given set of microstructural parameters. The presented example concerns application of* Al_2O_3-Cu *composite to brake disks.*

1 INTRODUCTION

The process of designing new materials in view of their future applications requires simultaneous effort of processing, characterization and modelling groups. In this paper we focus on the latter aspect. A general aim of the materials modelling is basically twofold. First, it is helpful in deeper understanding of the relations between composition, microstructure and effective properties of materials. Second, it can provide qualitative and quantitative predictions of a composite material behaviour before processing and experimental characterization of the composite. In those ways, the modelling supports the development of novel metal-ceramic composites for a variety of applications.

Our present goal is to develop an approach to find the optimal content of the phases in a metal-ceramic composite designed for specific purposes of a selected application. It is assumed that the application-directed requirements for the composite material are specified. Additionally, the processing method may impose constraints on the allowable compositions. The background of optimization procedures for finding a solution that fulfills multiple, conflicting objectives, as high thermal conductivity and a low coefficient of thermal expansion, has been described in [1, 2]. Following these ideas, we extend the approach to an enhanced set of thermo-mechanical properties of a two-phase composite. The overall thermo-mechanical properties of a composite can be predicted using the micromechanical approach. In this approach the overall response of a heterogeneous material is estimated on the basis of the knowledge of the phase properties by applying a selected averaging scheme. Potential applications of ceramic-metal Al_2O_3-Cu composite system to brake disks of desired properties, cf. [3], are studied.

2 MICROMECHANICAL MODELS

For estimation of linear effective properties of the metal-ceramic composites of perfectly bonded inclusions we use here simple Reuss (R) and Voigt (V) models, as well as Mori-Tanaka (MT) and self-consistent (SC) methods. Also upper and lower Hashin-Shtrikman (HS, SH) bounds are considered. It is worth to stress that closed-form solutions obtained within the V, R, HS, SH and MT schemes are particularly desirable for investigations of the best compositions by means of optimization methods. The above methods are well-known and described in detail elsewhere, e.g. in [12]. Therefore, only some basic formulae are quoted here.

In general, in linear theory of multiphase composites, the fourth-order overall stiffness tensor $\bar{\mathbf{L}}$ and the compliance tensor $\bar{\mathbf{M}}$ are established for the representative volume element and are expressed as follows

$$\bar{\mathbf{L}} = \sum_r c_r \mathbf{L}_r \mathbf{A}_r \,, \quad \bar{\mathbf{M}} = \sum_r c_r \mathbf{M}_r \mathbf{B}_r \,, \tag{1}$$

where $\mathbf{L}_r$ and $\mathbf{M}_r$ denote local stiffness and compliance tensors, respectively. Index r specifies the considered region of uniform properties while c_r is the volume content of this region in the representative volume. The fourth-order tensors $\mathbf{A}_r$ and $\mathbf{B}_r$ are so-called concentration tensors that relate local and averaged strains and stresses in a purely elastic problem. In the case of linear thermo-elasticity, the overall coefficient of thermal expansion $\bar{\boldsymbol{\alpha}}$, and the overall thermal conductivity tensor $\bar{\mathbf{k}}$ are calculated as follows [8, 12],

$$\bar{\boldsymbol{\alpha}} = \sum_r c_r \mathbf{B}_r^T \boldsymbol{\alpha}_r, \qquad \bar{\mathbf{k}} = \sum_r c_r \mathbf{k}_r \mathbf{a}_r \,, \tag{2}$$

where $\mathbf{k}_r$ is the local thermal conductivity for the phase r. The concentration tensor $\mathbf{a}_r$ relates local and average temperature gradients.

In the case of two-phase composites, the solutions for $\mathbf{A}_r$ and $\mathbf{a}_r$ are obtained considering only one inclusion, viz.:

$$\mathbf{A}_r = \left(\mathbf{I} + \mathbf{P}_r^0(\mathbf{L}_r - \mathbf{L}^0)\right)^{-1}, \qquad \mathbf{a}_r = \left(\mathbf{1} + \mathbf{p}_r^0(\mathbf{k}_r - \mathbf{k}^0)\right)^{-1}, \tag{3}$$

where $\mathbf{P}_r^0$ is the so-called polarisation tensor related to the Eshelby tensor and $\mathbf{I}$ is the fourth-order identity tensor. Analogously, $\mathbf{1}$ in the latter equation is the second-order identity tensor while $\mathbf{p}_r^0$ is the second-order tensor being the analog of the polarisation tensor for the elasticity problem. It depends on the shape of the ellipsoid and the matrix conductivity. The form of the Eshelby tensor for an ellipsoidal inclusion r is provided e.g. in [12]. For the self-consistent estimate the stiffness tensor $\mathbf{L}^0$ of the matrix is not known a-priori but it is derived as equal to the effective stiffness tensor $\mathbf{L}^0 = \bar{\mathbf{L}}$. In the case of Mori-Tanaka method $\mathbf{L}^0$ is the stiffness tensor of the matrix phase $\mathbf{L}^0 = \mathbf{L}_m$. The Hashin-Shtrikman bounds can be also obtained using the formulae (1) and (3).

The predictions of non-linear effective properties of metal matrix composites vary strongly depending on the method used. We have decided to adopt generalizations of the averaging methods selected for estimation of linear properties recalled above by employing the incremental linearization proposed in [5]. Two variants of the approach are employed that use either the tangent ($\mathbf{L}^t$) or secant ($\mathbf{L}^s$) current stiffness moduli [9]. From the point of view of the final goal to optimize composite properties, it is desirable to apply simple approaches of estimating the effective properties. Therefore, such approaches as the transformation field analysis [6], which requires numerical calculations of many influence tensors, the variational schemes [11] for which non-linear potentials describing the material behaviour have to be assumed or the FEM-methods which usually involve time-consuming calculations [10], have been evaluated as less suitable here.

The elasto-plastic behaviour of the metallic phase in a metal-matrix composite is usually identified by means of the stress-strain curve obtained in uniaxial tension or compression experiments. A procedure has been developed which enables to reconstruct the current secant or tangent stiffness of metallic phase directly on the basis of such a curve and use it as an input data in micromechanical analysis of the composite elasto-plastic response.

At this stage the behaviour of ceramic phase is assumed to be purely elastic, however it is possible to account for the damage development in this phase. For this purpose the concept of continuous damage mechanics can be used. In this context it is worth to notice that the use of the secant linearization enables softening of the phases to be considered.

3 OPTIMIZATION

A procedure for selection of optimal compositions of two-phase composite materials has been developed. Taking into account the key thermo-mechanical properties of the materials indicated by target applications and the advantages of the least square method, the multi-objective optimization problem has been formulated as follows:

Optimization problem: Find the optimal content of ceramic phase c_1 which minimises the following objective function

$$F(c_1) = \sum_{i=1}^{M} w_i \left(\frac{P_i^{\mathrm{eff}}(c_1)}{P_i^{\mathrm{des}}} - 1 \right)^2 \tag{4}$$

subject to the constraints

$$c_1^- \leq c_1 \leq c_1^+ , \quad P_i^{\mathrm{tar}-} \leq P_i^{\mathrm{eff}}(c_1) \leq P_i^{\mathrm{tar}+} . \tag{5}$$

In the above formula M is the number of properties to be optimized, P_i^{eff} is the effective property i of the composite while P_i^{des} is the desired value of property i in view of the application. A property is represented by its direct physical value or its inverse so that the effective and desired values of a property satisfy $P_i^{\mathrm{eff}} \leq P_i^{\mathrm{des}}$. The value of P_i^{des} is taken as $P_i^{\mathrm{des}} = \max P_i^{\mathrm{eff}}(c_1)$ subject to (5). The first inequalities express the limitation imposed by processing condition on the achievable content of ceramic phase. In the second constraint inequalities, $P_i^{\mathrm{tar}-}$ and $P_i^{\mathrm{tar}+}$ denote lower and upper bounds to property i imposed by the project targets and phase properties. Scalars w_i are the weight assigned to property i for the application under consideration.

For solving the optimization problem a computer code implemented within the *Wolfram Mathematica* package has been developed.

4 APPLICATION

The following key properties have been indicated for the material for a brake disk:

- reduced specific weight, ρ,
- high stiffness (high Young's modulus, E),
- high strength (ultimate tensile/compressive stress, UTS),
- enhanced thermal conductivity, TC,
- lower thermal expansion, CTE.

Other practically important properties like enhanced resistance to high temperature and resistance to wear and corrosion are more difficult to be quantified, and therefore are not included in the calculations. As basic microstructural parameter we will consider volume fraction of ceramic inclusions.

Within the MATRANS European project [1] certain limits to the above properties have been indicated by comparison with the corresponding characteristics of gray cast iron as the reference material nowadays used in the automotive industry for brake disks [4, 7]. Namely, $\bar{\alpha} < 12 \cdot 10^{-6}\,\mathrm{K}^{-1}$ (CTE), $\bar{k} \geq 77\,\mathrm{W/m \cdot K}$ (TC), $\rho < 7.25\,\mathrm{g/cm^3}$, $\mathrm{UTS} > 255\,\mathrm{MPa}$. As a possible alternative, Al_2O_3-Cu composite with alumina content $0.2 \leq c_1 \leq 0.8$ has been selected.

The first step of the analysis has been the verification whether the proposed composite system is potentially capable to fulfill the requirements imposed on effective thermo-mechanical properties. Using the literature data for individual phases, the linear isotropic effective properties of Al_2O_3-Cu composite, i.e. Young's and shear moduli, coefficients of thermal expansion

[1] see Projects/Matrans at www.kmm-vin.eu

and thermal conductivity have been computed as functions of volume fraction of the ceramic phase using the methods outlined in Section 2. The results concerning the coefficient of thermal expansion (CTE) and thermal conductivity (TC) are presented in Fig. 1. The calculations have been performed under the assumption of spherical shape of inclusions, overall isotropy and perfect bonding.

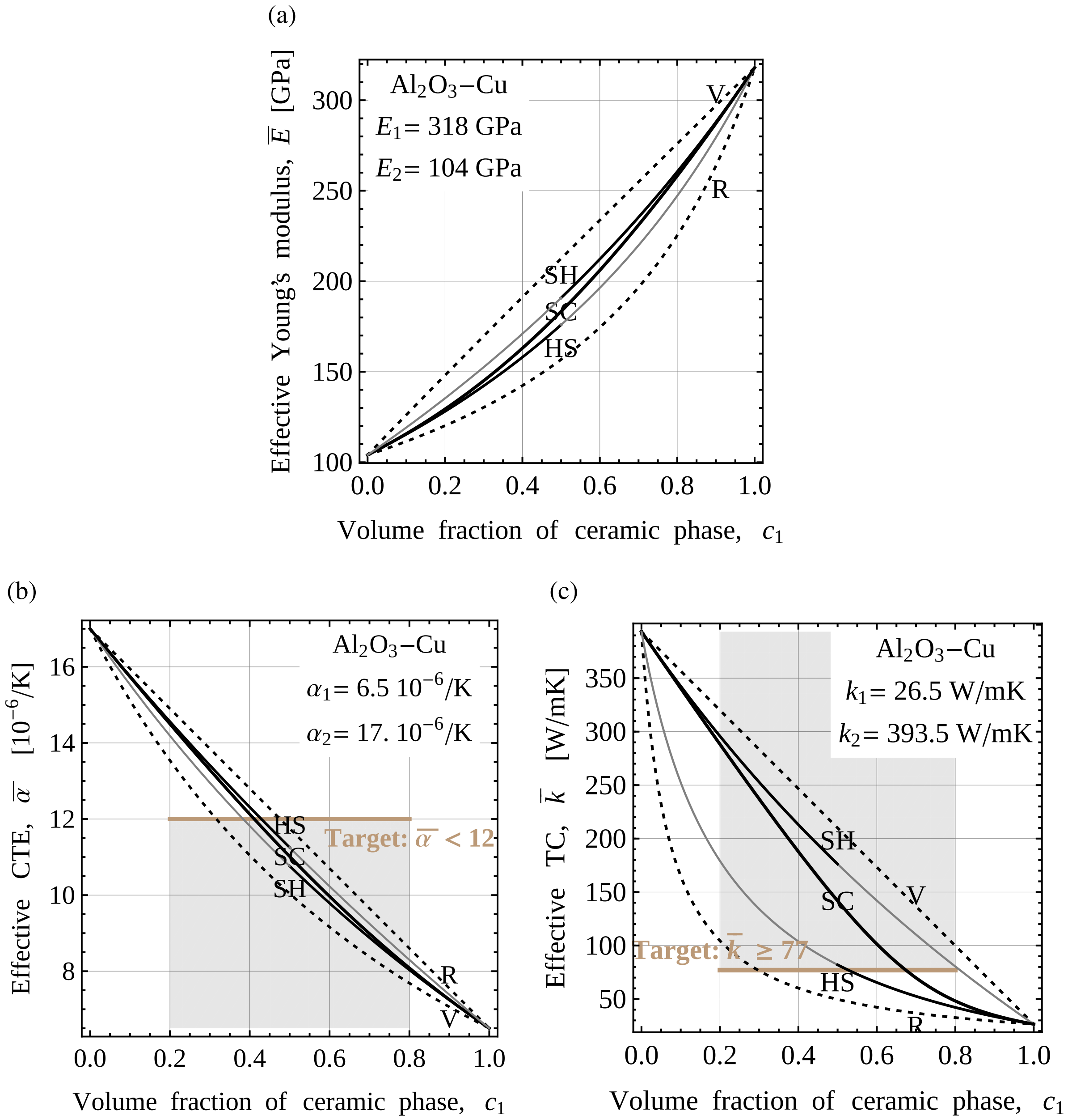

Figure 1: Effective Young's modulus $\bar{E}$ (a), coefficient of thermal expansion (CTE) (b) and thermal conductivity (TC) (c) for Al_2O_3-Cu composite as functions of volume fraction of the ceramic phase, determined by several micromechanical models.

The analysis indicates that the project targets may be achieved, and that the best theoretical estimate from those examined for linear properties, lying between the bounds, is provided by the self-consistent (SC) method. Regarding non-linear mechanical properties, both HS and SC methods for the secant and tangent schemes predict that the requirement $\mathrm{UTS} > 255\,\mathrm{MPa}$ can be satisfied for $c_1 > 0.2$ for a reference stress-strain curve for Cu in the plastic range (Fig. 2).

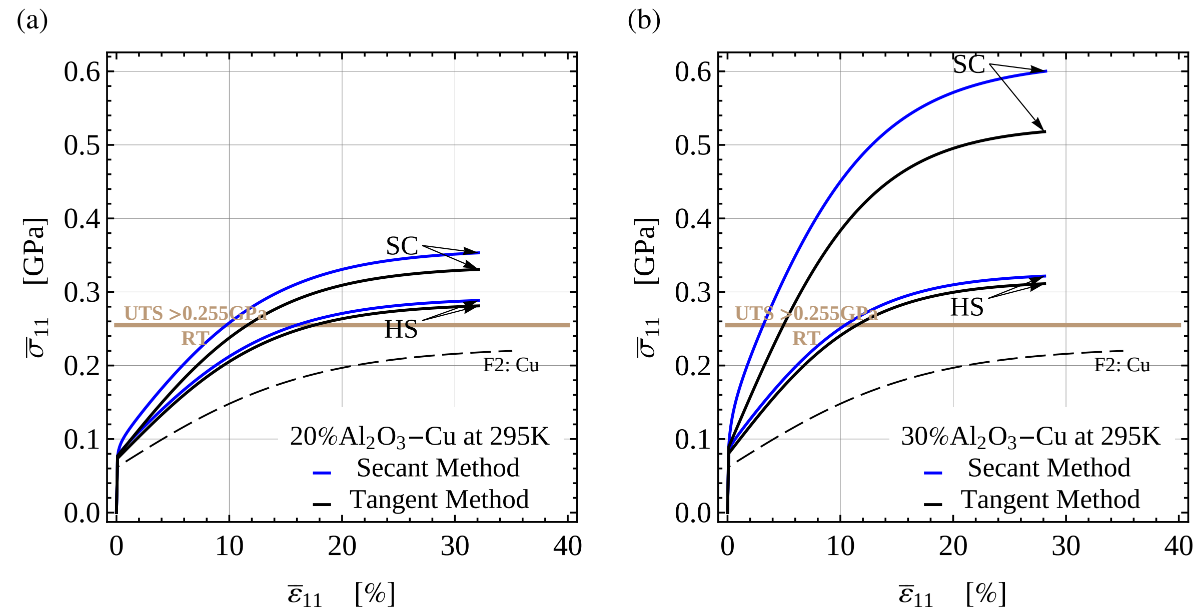

Figure 2: Effective stress-strain curve for Al_2O_3-Cu composite.

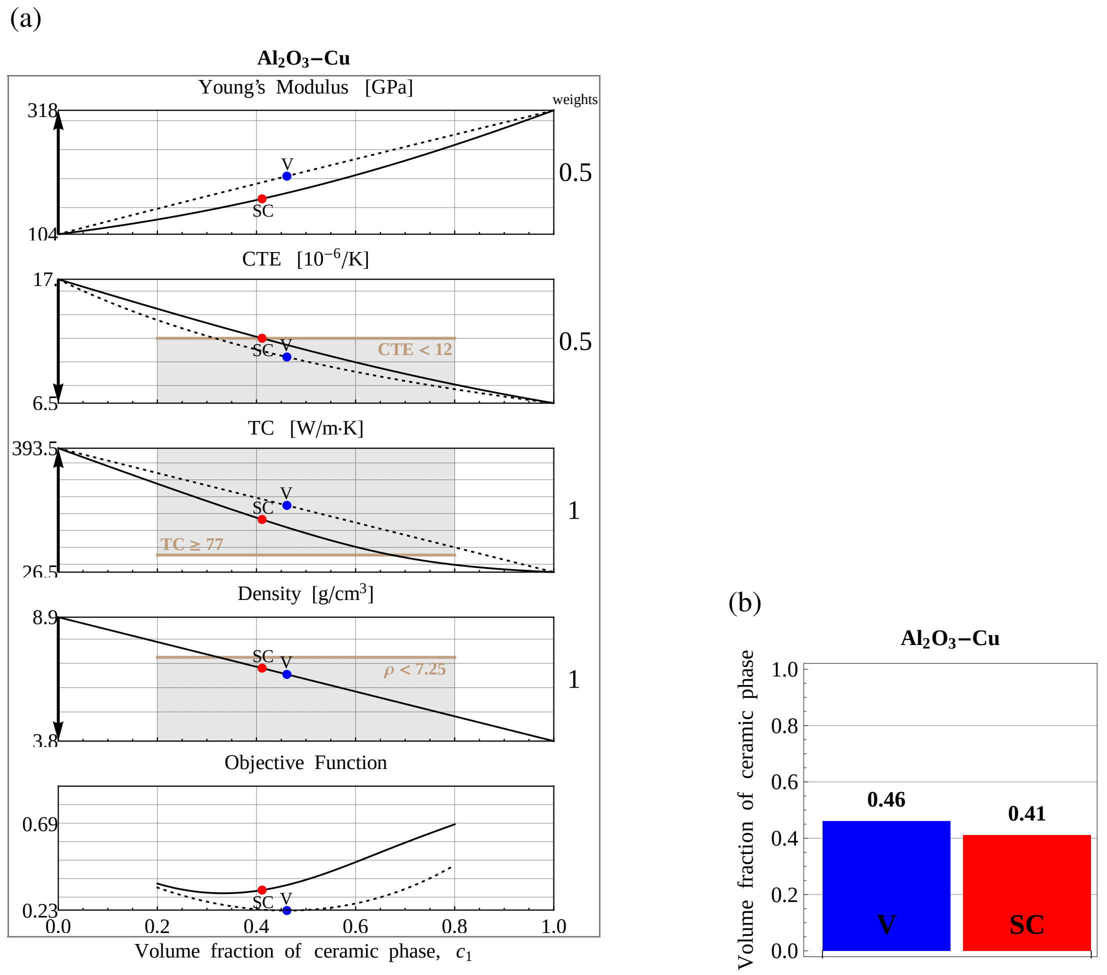

Figure 3: Estimation of optimal content of ceramic phase in Al_2O_3-Cu for brake disk application.

This conclusion is only qualitative since the actual stress-strain curve for Cu can be significantly influenced by the processing method, e.g., powder metallurgy.

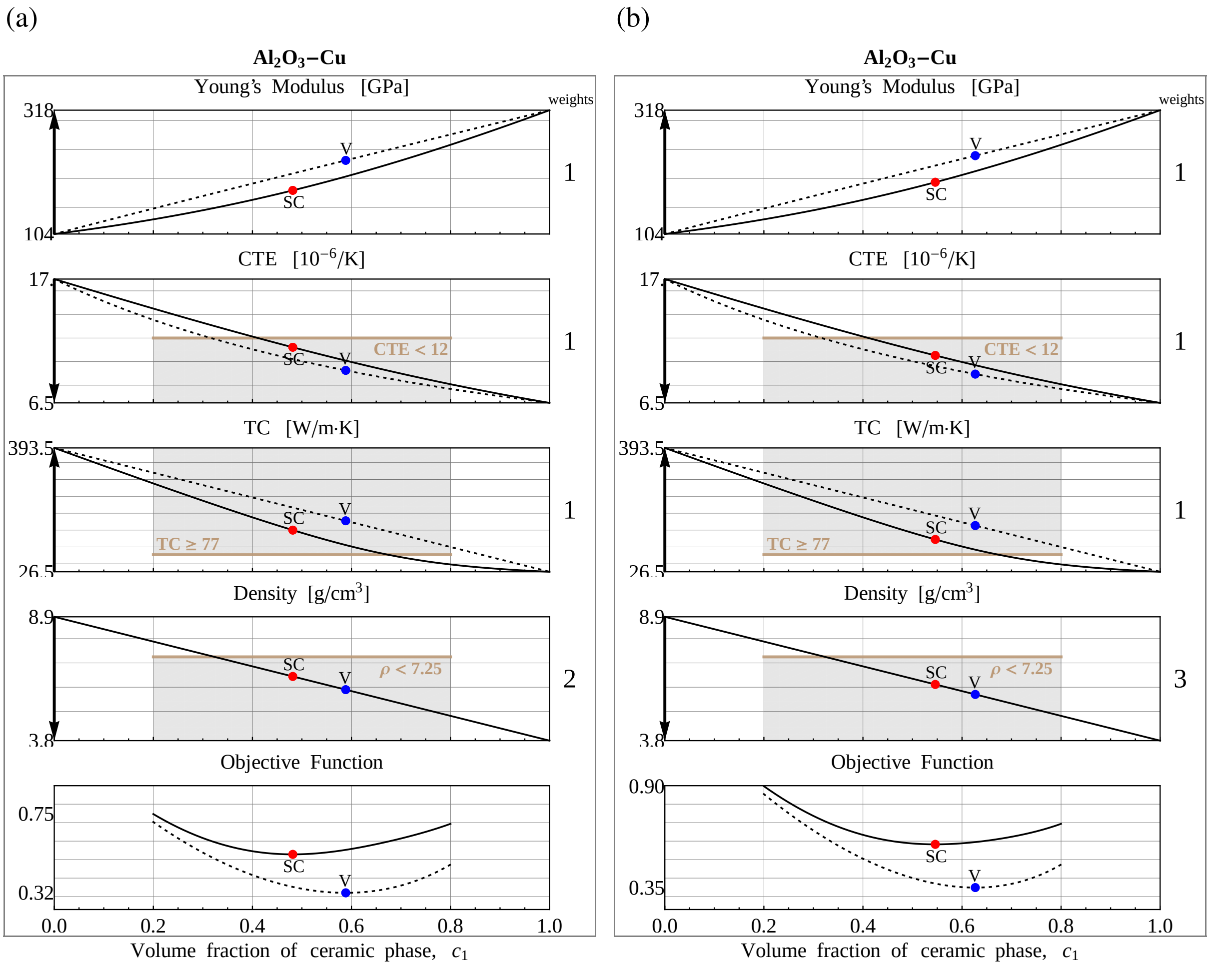

Figure 4: Dependence of the estimated optimal content of ceramic phase on weights w_i reflecting the importance of the considered property i for brake disk application.

By applying the optimization procedure outlined in Section 3, optimal content of ceramic phase has been found for the selected application. In Fig. 3 estimation of optimal content c_1 (block diagram) of the Al_2O_3 phase in composite Al_2O_3-Cu is illustrated for low density, high TC, low CTE and high stiffness under the constraints imposed by project targets for brake disk. The shaded area represents the domain allowable by the project targets and production limitations. The lowest diagram corresponds to the objective function defined by (4), the next one is the theoretical density function, and three next diagrams are calculated as in Fig. 1. Bold points on the diagrams correspond to the optimal content c_1 determined by using two different methods of calculation of effective properties (V - Voigt, SC - self-consistent). Comparison of Figs. 3a and 4a,b shows how the optimization results can be influenced by the choice of weights assigned to the subsequent properties in the objective function (4). In Fig. 4 the weights have been assigned to increase the importance of low density.

5 CONCLUSIONS

Although not all properties desirable in the application considered could have been taken into account in the present optimization procedure due to insufficient data, some major conclusions can be drawn as follows:

- The procedure developed for predicting optimal compositions of two-phase composites taking into account the key thermo-mechanical properties with weight factors specified for a selected application works effectively for several conflicting objectives.
- From various micromechanical approaches used to determine overall properties of the composite, the self-consistent approach (SC) appears to be most reliable.
- The optimization result (ceramic content 41%) is affected by the limit imposed on the coefficient of thermal expansion (CTE) for the choice of weight factors as in Fig 3a.
- If the weights are taken to emphasize the importance of low density, as in Fig. 4, then the optimal ceramic content increases and the CTE limit becomes inactive.

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