SENSITIVITY ANALYSIS FOR EFFECTIVE PROPERTIES OF PERIODIC FIBER-REINFORCED COMPOSITES

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ABSTRACT

Computational sensitivity analysis of effective elasticity tensors for various fiber-reinforced periodic composite structures is the main aim of this paper. Homogenization method based on the Finite Element Method solution of the cell problems is employed to compute effective properties. Thanks to the finite difference scheme the sensitivity gradients are calculated next to compare the influence of various material parameters on effective tensor components for different combinations of the components. The results obtained confirm that for most combinations of various fibers and matrices the most decisive material parameters are Poisson's ratio of the matrix and Young modulus of the fiber. The methodology can be used together with the appropriate cost function to optimise the materials choice for a specific composite design.

1. INTRODUCTION

Effective properties of composites are usually determined to speed up a designing process of new engineering heterogeneous materials by a reduction of a computational model to the macro scale only. It is done using homogenization method [2,4,6-8,10-11], where the Finite Element Method (FEM) solution for the cell problem solved on the Representative Volume Element (RVE) is employed to approximate global characteristics of composites. This methodology can be relatively easy adopted in sensitivity analysis [4,7] enabling optimization of composites properties according to the specific design constraints.

Sensitivity analysis of effective composite characteristics is the main subject of numerical studies carried out below by the computer system MCCEFF in conjunction with the Central Finite Difference scheme. The program is based on the FEM plane strain analysis, where in-plane effective characteristics for deterministic composites are computed. Sensitivity gradients of the homogenized material characteristics are determined for various engineering fiber-reinforced composites with respect to elastic characteristics of the components. Further, the functionals of strain energy are defined for uniaxial, biaxial, transverse as well as for a combined biaxial/transverse strain states applied at the periodicity cell. Their gradients are calculated using special combinations of sensitivity coefficients for the homogenized elasticity tensor components. The comparison of all these coefficients makes it possible to determine the most decisive material parameters for various types of the fiber-reinforced structures having carbon, steel or graphite fibers and polymer-based matrices under various loadings.

Further extensions of the methodology proposed are discussed in terms of multicomponent periodic composites [6,8,11], sensitivity analysis in homogenization of coupled multiphysics and, on the other hand, multiscale problems as well as in case of heterogeneous structures with randomly defined material properties [7].

2. THEORETICAL BACKGROUND

Let us consider a periodic composite in plane strain in initially unstressed and undeformed state with the cross-section constant along x_3 axis. Let us assume that the RVE denoted by Ω of Y contains the fiber and the matrix such that

$$\Omega = \Omega_1 \cup \Omega_2 \cup \Gamma_{12} = \partial\Omega_{12}, \quad (1)$$

$$\Omega_1 \cap \Omega_2 = \varnothing, \quad (2)$$

where Γ_{12} is the interface between the components. The example of such a structure with rectangular external boundary is shown in Fig. 1 with the RVE (periodicity cell) - in Fig. 2.

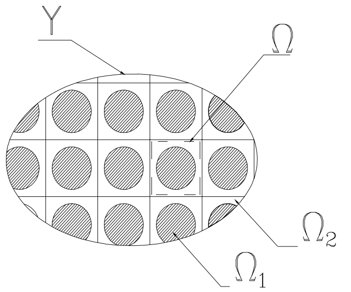

Fig. 1. Plane composite structure.

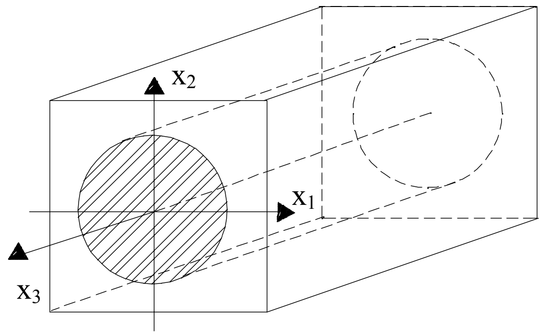

Fig. 2. The RVE in 3D view.

Let any component of the composite be a linear-elastic transversely isotropic material defined by its Young modulus and Poisson's ratio

$$e(\mathbf{x}) = \gamma_a(\mathbf{x})\cdot e_a, \quad \nu(\mathbf{x}) = \gamma_a(\mathbf{x})\cdot \nu_a, \text{ for a=1,2; } \mathbf{x}\in\Omega, \tag{3}$$

with γ_a being a characteristic function

$$\gamma_a(x) = \begin{cases} 1, x\in\Omega_a \\ 0, x\in\Omega/\Omega_a \end{cases}, \text{ for a=1,2; } \mathbf{x}\in\Omega. \tag{4}$$

Then, the elasticity tensor field $C_{ijkl}(\mathbf{x})$ is defined as

$$C_{ijkl}(\mathbf{x}) = e(\mathbf{x})\left\{\delta_{ij}\delta_{kl}\frac{\nu(\mathbf{x})}{(1+\nu(\mathbf{x}))(1-2\nu(\mathbf{x}))} + \left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)\frac{1}{2(1+\nu(\mathbf{x}))}\right\}, \tag{5}$$

i,j,k,l=1,2.

The effective elasticity tensor $C^{(eff)}_{ijkl}$ is obtained from a solution of the following boundary problem [2,6-8,10]:

$$-\operatorname{div}\left(\mathbf{C}^{\delta}\boldsymbol{\varepsilon}\left(u^{\delta}\right)\right)=\mathbf{f}, \ \mathbf{x}\in\Omega \tag{6}$$

$$\varepsilon_{ij}\left(\mathbf{u}^{\delta}\right)=\tfrac{1}{2}\left(u^{\delta}_{i,j}+u^{\delta}_{j,i}\right), \ \mathbf{x}\in\Omega \tag{7}$$

$$\mathbf{C}^{\delta}=\gamma^{\delta(a)}(x_i)\mathbf{C}^{\delta(a)}, \ \mathbf{x}\in\Omega, \text{ a=1,2,} \tag{8}$$

and the periodic boundary conditions

$$\mathbf{u}^{\delta}(x_i) = \mathbf{u}^{\delta}(x_i + l_i); \ \mathbf{x}\in\partial\Omega, \tag{9}$$

l_i for i=1,2 denote the dimension of the RVE in x_i direction.

The quantity δ, called a geometrical scale parameter, relates the dimensions of the RVE to the corresponding dimensions of the entire composite structure; the same number of periodicity cells in horizontal and vertical directions follows the assumption about such a parameter existence. Displacement $\mathbf{u}^{\delta}$ is as a solution of this problem obtained using classical variational methods and taking the limit with $\delta \to 0$ called $\mathbf{u}^{0}$, employed to determine effective tensor.

The following stress boundary conditions are imposed at the interfaces between the constituents, to determine the homogenization function [7,8]:

$$\sigma_{ij}\left(\chi^{(pq)}\right)n_j = \left[C_{ijpq} \right]\Big|_{\Gamma_{12}} n_j = F_i^{(pq)}\Big|_{\Gamma_{12}} \; ; \; \mathbf{x} \in \Gamma_{12}, \tag{10}$$

where n_j is the component of a unit vector normal to the corresponding interface and directed to the RVE interior. Moreover, $\left[C_{ijpq} \right]\Big|_{\Gamma_{12}}$ denote the difference of the elasticity tensor components values for the components applied at this interface. Then, integral statement for the homogenization problem can be proposed as

$$\int_{\Omega} C_{ijkl}\, \varepsilon_{kl}\left(\chi^{(pq)}\right)\varepsilon_{ij}(\mathbf{v})\, d\Omega = \int_{\Gamma_{12}} \left[C_{ijpq} \right]\Big|_{\Gamma_{12}} n_j v_i \, d\Gamma, \tag{11}$$

which makes it possible to compute the functions $\chi^{(11)}$, $\chi^{(12)}$ and $\chi^{(22)}$. After some algebra the effective elasticity tensor components are calculated as follows:

$$C_{ijpq}^{(eff)} = \frac{1}{|\Omega|} \int_{\Omega} \left(C_{ijpq} + C_{ijkl}\varepsilon_{kl}\left(\chi^{(pq)}\right)\right) d\Omega = \left\langle C_{ijpq} \right\rangle_{\Omega} + \left\langle C_{ijkl}\varepsilon_{kl}\left(\chi^{(pq)}\right)\right\rangle_{\Omega}. \tag{12}$$

As it is known, structural design sensitivity analysis is useful in common application with various discrete numerical techniques for the boundary problems solutions and in implementation into the relevant computer programs. This analysis is essentially more complicated in the case of homogenization method, because the effective characteristics of a composite material and/or structure are determined first and the design process is related to the homogenized system discretized in the macro-scale only. Sensitivity analysis in case of homogenization procedure is equivalent to verification of the effective elasticity tensor gradients with respect to material parameters of the constituents as well as volume ratios of composite constituents, etc. These gradients to the sensitivity parameters vector represented by **h** can be calculated as

$$\frac{dC_{ijpq}^{(eff)}}{d\mathbf{h}} = \frac{\partial}{\partial \mathbf{h}} \left\{ \frac{1}{|\Omega|} \int_{\Omega} C_{ijpq}\, d\Omega \right\} + \frac{\partial}{\partial \mathbf{h}} \left\{ \frac{1}{|\Omega|} \int_{\Omega} C_{ijkl}\varepsilon_{kl}\left(\chi_{(pq)}\right) d\Omega \right\}, \tag{13}$$

which can be further rewritten as

$$\frac{dC_{ijpq}^{(eff)}}{d\mathbf{h}} = \frac{1}{|\Omega|} \int_{\Omega} \frac{\partial C_{ijpq}}{\partial \mathbf{h}} d\Omega + \frac{1}{|\Omega|} \int_{\Omega} \frac{\partial C_{ijkl}}{\partial \mathbf{h}} \varepsilon_{kl}\left(\chi_{(pq)}\right) d\Omega + \frac{1}{|\Omega|} \int_{\Omega} C_{ijkl} \frac{\partial \varepsilon_{kl}\left(\chi_{(pq)}\right)}{\partial \mathbf{h}} d\Omega. \tag{14}$$

It is necessary to underline that differentiation with respect to any design sensitivity parameter can be inserted under the integration sign over the RVE, if only geometrical sensitivity is not considered. That is why the last component from Eq. (14) need to be computed by the finite difference calculus, i.e.

$$\frac{\partial C^{(\mathrm{eff})}_{\alpha\beta\gamma\delta}}{\partial h^{d}} \cong \frac{1}{\varepsilon}\left[C^{(\mathrm{eff})}_{\alpha\beta\gamma\delta}\left(h^{d} + 1_{d}\,\varepsilon\right) - C^{(\mathrm{eff})}_{\alpha\beta\gamma\delta}\left(h^{d}\right)\right],\ \overline{d} = 1,2,...,D, \tag{15}$$

where h^{d} is the d-th component of the D-dimensional design variable vector h, ε represents a small perturbation and the D-dimensional vector 1_{d} is equal to 1 for d-th component of the design variables vector and zeroes elsewhere.

Since the sensitivity coefficients should be comparable with each other to distinguish the crucial design parameter, the function analyzed is normalized with respect to the derivation parameter and hence the following normalization rule is applied [7,9]

$$\left(\frac{dC^{(\mathrm{eff})}_{ijpq}}{d\mathbf{h}}\right)_{\mathrm{scaled}} = \frac{\partial C^{(\mathrm{eff})}_{ijpq}}{\partial \mathbf{h}} \cdot \frac{h}{C^{(\mathrm{eff})}_{ijpq}(h)} \text{ (no summation over I,j,p,q).} \tag{41}$$

Now, let us focus on the last component of Eq. (14) containing sensitivity gradients of homogenization function. The basic equilibrium equation to solve for this function is generally represented in the FEM description as [1,9,13]

$$K_{\alpha\beta}\left(\mathbf{h}^{(\mathrm{eff})}\left(h^{d}\right); h^{d}\right)\chi^{pq}_{\beta}\left(\mathbf{h}^{(\mathrm{eff})}\left(h^{d}\right); h^{d}\right) = Q^{pq}_{\alpha}\left(\mathbf{h}^{(\mathrm{eff})}\left(h^{d}\right); h^{d}\right) \tag{17}$$

where design parameters influence the homogenized characteristic, or alternatively

$$K_{\alpha\beta}\left(\mathbf{h}^{(\mathrm{eff})}; h^{d}\right)\chi^{pq}_{\beta}\left(\mathbf{h}^{(\mathrm{eff})}; h^{d}\right) = Q^{pq}_{\alpha}\left(\mathbf{h}^{(\mathrm{eff})}; h^{d}\right). \tag{18}$$

The second case reflects the situation, where the homogenized composite plate with its arbitrarily constant thickness as the design variable is considered [10].

The SDS analysis of homogenized structure is quite similar to traditional structural sensitivity modeling [5,9] of a composite except the fact that homogenized parameters are to be pre-calculated and inserted into a single additional vector h^{d}. This is the case, where external load vector (or its location) is original design parameter and, at the same time, effective Young modulus is to be taken as the extra sensitivity parameter. Let us mention that sometimes, the real composite is built from isotropic but contrastively different materials whereas homogenized structure is homogeneous but orthotropic, which needs the finite element type redefinition during the FEM meshing (finite element type change) and the new solution, etc.

Numerical methodology changes however for Eq. (18), which illustrates the case, where homogenized composite is tested numerically and elastic characteristics of its components are chosen as design parameters. Then, effective properties being the parameters of final state functions are some functions of these elastic characteristics. Hence, differentiation process in modification of Eq. (18) is modified to

$$K_{\alpha\beta}\left(h^{d}\right)\frac{\partial \chi^{pq}_{\beta}\left(h^{d}\right)}{\partial \mathbf{h}^{(\mathrm{eff})}}\frac{\partial \mathbf{h}^{(\mathrm{eff})}}{\partial h^{d}} = \frac{\partial Q^{pq}_{\alpha}\left(h^{d}\right)}{\partial \mathbf{h}^{(\mathrm{eff})}}\frac{\partial \mathbf{h}^{(\mathrm{eff})}}{\partial h^{d}} - \frac{\partial K_{\alpha\beta}\left(h^{d}\right)}{\partial \mathbf{h}^{(\mathrm{eff})}}\frac{\partial \mathbf{h}^{(\mathrm{eff})}}{\partial h^{d}}\chi^{pq}_{\beta}\left(h^{d}\right). \tag{19}$$

This equation reduces in case of

$$\frac{\partial Q_{\alpha}^{pq}\left(h^{d}\right)}{\partial \mathbf{h}^{(eff)}} = 0\,, \tag{20}$$

to the following formula:

$$K_{\alpha\beta}\left(h^{d}\right)\frac{\partial \chi_{\beta}^{pq}\left(h^{d}\right)}{\partial \mathbf{h}^{(eff)}}\frac{\partial \mathbf{h}^{(eff)}}{\partial h^{d}} = -\frac{\partial K_{\alpha\beta}\left(h^{d}\right)}{\partial \mathbf{h}^{(eff)}}\frac{\partial \mathbf{h}^{(eff)}}{\partial h^{d}}\chi_{\beta}^{pq}\left(h^{d}\right). \tag{21}$$

The most interesting problem, however, is not to determine the sensitivity coefficients of the homogenized tensor with respect to particular composite parameters, but to approximate the sensitivity of the entire homogenized composite structure under general boundary conditions to some of its design parameters similarly to considerations dealing with homogeneous systems provided in [5,9]. Therefore, let us introduce the sensitivity functional as the strain energy of the homogenized composite under some combination of the uniform constant strains in x and y directions as well as for the transverse strain ε_{xy} as it is illustrated below (cf. Fig. 3). In this case, the sensitivity functional is obtained as

$$\begin{aligned} G &= \tfrac{1}{2}\int_{\Omega}\left(\{C_{1111}^{(eff)}\varepsilon_{11} + C_{1122}^{(eff)}\varepsilon_{22}\}\,\varepsilon_{11} + \{C_{1212}^{(eff)}\varepsilon_{12} + C_{1221}^{(eff)}\varepsilon_{21}\}\,\varepsilon_{12}\right)d\Omega + \\ &+ \tfrac{1}{2}\int_{\Omega}\left(\{C_{2121}^{(eff)}\varepsilon_{21} + C_{2112}^{(eff)}\varepsilon_{12}\}\,\varepsilon_{21} + \{C_{2211}^{(eff)}\varepsilon_{11} + C_{2222}^{(eff)}\varepsilon_{22}\}\,\varepsilon_{22}\right)d\Omega \end{aligned} \tag{22}$$

The strain state relevant to this functional contains uniform extension of the RVE both in horizontal and vertical directions as well as under its uniform shear. It can result in (a) uniaxial compression/tension of the RVE: $\varepsilon_{11} = 1, \varepsilon_{12} = 0, \varepsilon_{22} = 0$

$$G_{u} = \frac{l^{2}}{2}\left(C_{1111}^{(eff)}\right), \tag{23}$$

(b) biaxial compression/tension of the RVE: $\varepsilon_{11} = 1, \varepsilon_{12} = 0, \varepsilon_{22} = 1$

$$G_{b} = l^{2}\left(C_{1111}^{(eff)} + C_{1122}^{(eff)}\right), \tag{24}$$

(c) shear (or torsion) of the composite specimen: $\varepsilon_{12} = 1, \varepsilon_{\alpha\alpha} = 0$

$$G_{t} = 2l^{2}\left(C_{1212}^{(eff)}\right) \tag{25}$$

or some mixed strain state for the homogenized material, where l is a basic dimension of the square RVE cell. Eq. (23) should be represented by two independent formulas for uniaxial strain along x_1 and x_2 axes when the fiber is flattened to the ellipsoidal cross-section and where its semi-axes coincide with the RVE coordinates. Further, let us note that the difference between these strain tensor components is important in all cases, where the cell is subjected to the unsymmetric strain field (transverse strain dominates over biaxial strains or $\varepsilon_{11}>\varepsilon_{22}$). Integrating over the RVE domain, recalling assumed constant strain over this cell as well as constant character of $C_{ijkl}^{(eff)}$ on Ω, one can get thanks to the elasticity tensor symmetry as

$$G = l^2\left(C_{1111}^{(eff)} + C_{1122}^{(eff)} + 2C_{1212}^{(eff)}\right). \tag{26}$$

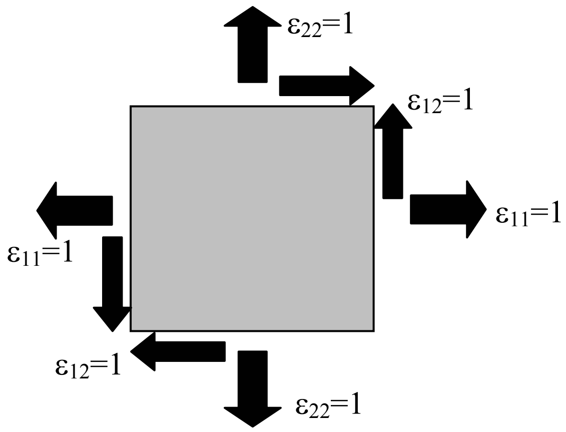

Fig. 3. Graphical representation of the generalized strain state on the RVE.

Finally, partial derivatives of G with respect to any component of the design parameters vector **h** can be calculated as

$$G^{,h} = \frac{\partial G}{\partial \mathbf{h}} = l^2\left\{\frac{\partial C_{1111}^{(eff)}}{\partial \mathbf{h}} + \frac{\partial C_{1122}^{(eff)}}{\partial \mathbf{h}} + 2\frac{\partial C_{1212}^{(eff)}}{\partial \mathbf{h}}\right\}. \tag{27}$$

Using this formula, the most important design parameter for the homogenized composite in uniform plane strain can be determined using the effective elasticity tensor gradients determined from Eq. (13).

3. RESULTS & DISCUSSION

Let us consider a composite with periodicity cell shown below - the fiber has round cross-section and the entire cell is rectangular. The composite analyzed is perfectly periodic, fibers are distributed uniformly in the transverse cross-section, while the reinforcement ratio is equal to 50% of the total area of the RVE. The following material characteristics are adopted [12] to carry out the sensitivity analysis for various fiber-reinforced composites: C/epoxy, glass/epoxy, C/PEEK, glass/PEEK, B/Ti, SiC/Ti, Al_2O_3/Ti, C/Al, C/Mg and C/Borosilicate glass; the FEM discretization using 4-node linear rectangular plane strain elements [1,13] implemented in the system MCCEFF is presented in Fig. 4.

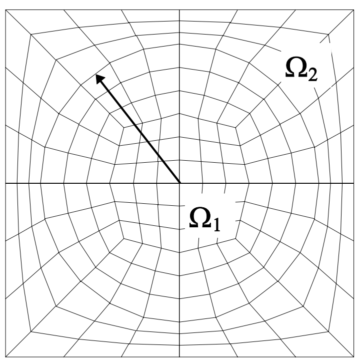

Fig. 4. FEM discretization of the periodicity cell.

Table 1. Typical properties of the components.

Material	Young modulus [GPa]	Poisson's ratio
C	84,0	0,22
Glass	71,0	0,22
B	420,0	0,20
SiC	406,0	0,20
Al_2O_3	385,0	0,20
Epoxy	3,50	0,33
PEEK	4,00	0,37
Ti	113,8	0,33
Al	69,0	0,33
Mg	45,5	0,33
Borosilicate glass	63,7	0,21

Table 2. Effective properties of the analyzed composites.

Composite type	$C^{(eff)}_{1111}$ [GPa]	$C^{(eff)}_{1122}$ [GPa]	$C^{(eff)}_{1212}$ [GPa]
B/Ti	266.425	96.438	107.548
SiC/Ti	262.897	95.398	104.691
Al_2O_3/Ti	257.365	93.748	100.405
C/Al.	98.365	38.626	30.097
C/Borosilicate glass	82.538	22.474	30.292
C/Mg	79.690	31.072	25.590
C/PEEK	17.071	6.414	17.608
Glass/PEEK	16.546	6.292	14.998
C/Epoxy	13.376	4.228	17.535
Glass/Epoxy	12.990	4.155	14.925

The results of initial homogenization analysis are contained in Table 2 for various combinations of the fibers and the matrices from Table 1. These results agree with an engineering intuition that the larger composite components are the higher effective elasticity tensor components are obtained. Further it is seen by a comparison with Table 1 that the homogenized characteristics computed are significantly smaller than the additional spatial averages of the elasticity tensor over the RVE. Contrasting the largest and the smallest values of the effective tensor it can be concluded that the highest contrast is obtained for the component $C^{(eff)}_{1122}$ (about 23 times), then for $C^{(eff)}_{1122}$ (more than 20 times) and for $C^{(eff)}_{1122}$ (almost 7 times only).

The results of computational sensitivity studies are collected in Figs. 5-8: the sensitivity gradients for strain energy functionals in uniaxial (dGudh), biaxial (dGbdh), transverse (dGtdh) and general strain states (dGdh) of the RVE are collected adopting Young modulus of the fiber (Fig. 5), of the matrix (Fig. 6) as well as Poisson's ratios of the fiber (Fig. 7) and the matrix (Fig. 8) as successive design parameters.

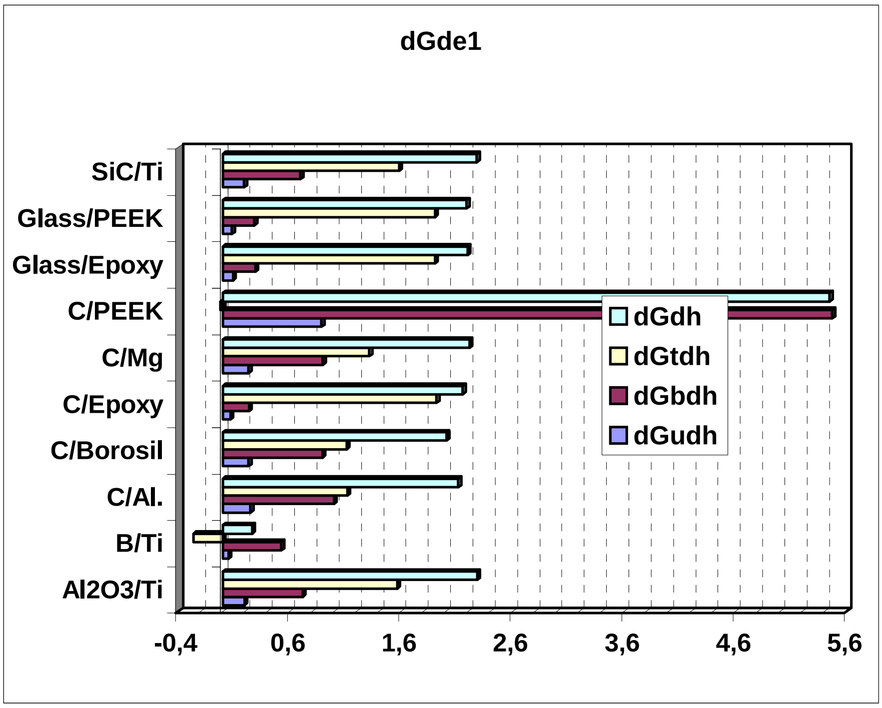

Fig. 5. Sensitivity gradients for **h**≡e_1.

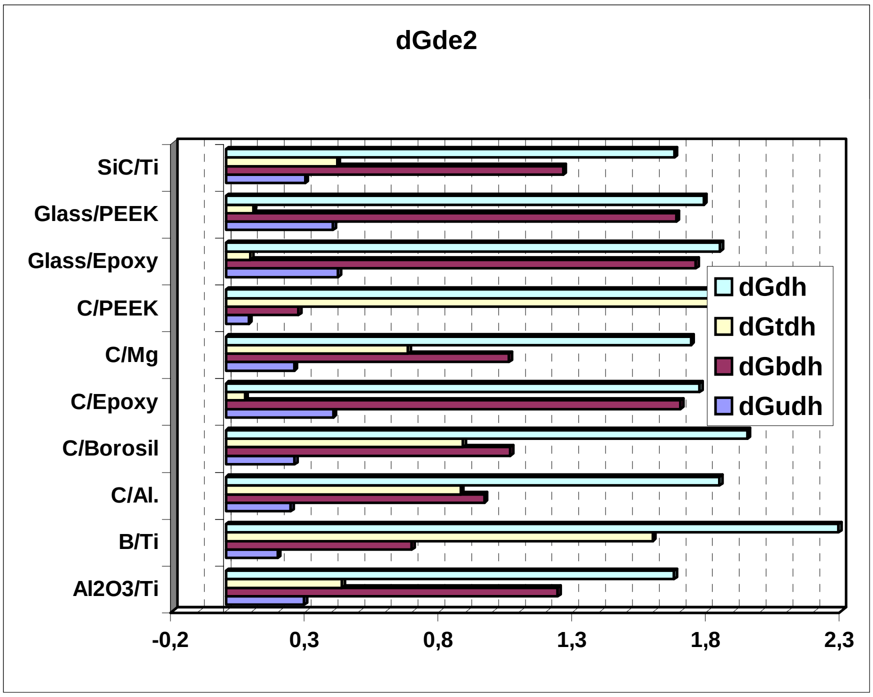

Fig. 6. Sensitivity gradients for **h**≡e_2.

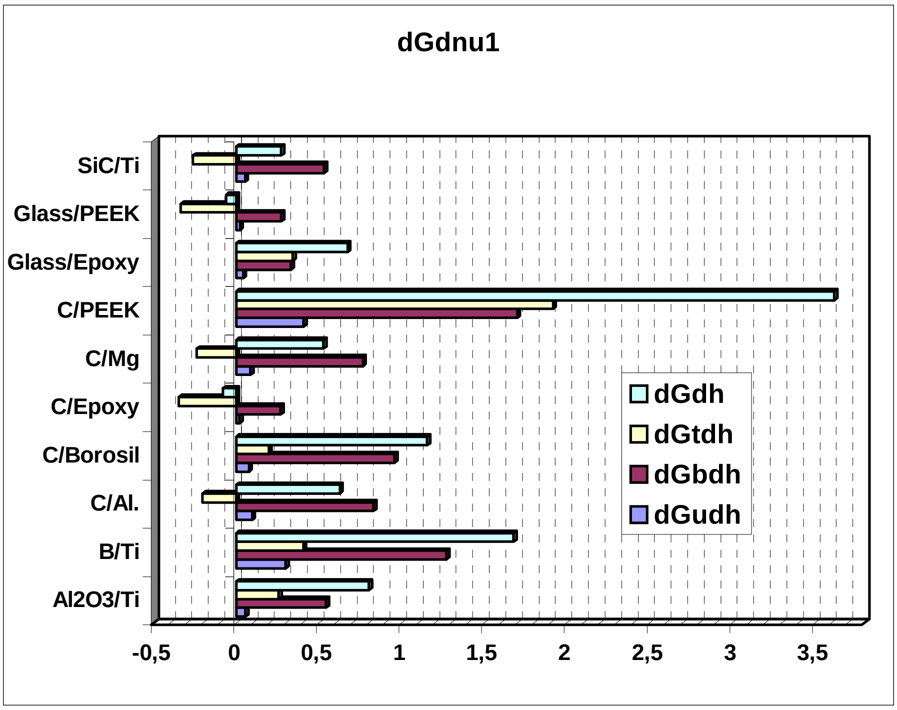

Fig. 7. Sensitivity gradients for **h**≡ν_1.

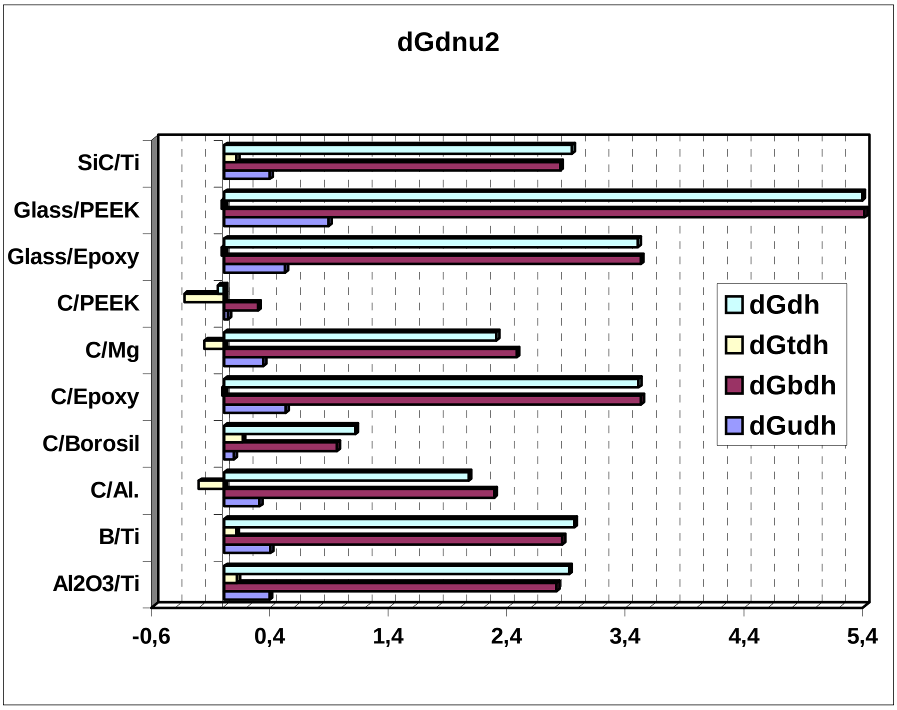

Fig. 8. Sensitivity gradients for **h**≡ν_2.

General conclusion is that the Poisson's ratio of the matrix and Young modulus of the fiber are the most decisive material parameters for all these composites. The remaining material parameters are less important for the overall response of the RVE in various strain states verified. Two cases – B/Ti and C/PEEK violate this rule, where Young modulus of the matrix is more decisive in the first example; the Poisson's ratio of the fiber is crucial for the second composite. Further, it is seen that most of sensitivity gradients are positive. Some negative values are obtained for Poisson's ratios as design variables and the single exception in the case of Young modulus of the fiber (B/Ti composite). Let us note that the negative gradients appear almost only in transverse strain imposed on the RVE.

4. CONCLUDING REMARKS

Poisson's ratio of the matrix and Young modulus of the fiber have been verified as the most decisive material parameters for the effective elastic parameters and the strain energy of the RVE in a combination of biaxial and transverse strain states. It confirms previous results obtained for C/Epoxy composite in [7]. Some small exceptions from this rule have been observed, too. Numerical methodology leading to these conclusions, enriched with the relevant algorithm based on some specific cost function, may enable engineering optimization of various composites.

Further computational studies are however necessary to check the influence of reinforcement volume fraction on the results of homogenization because various material combinations need different value of this fraction. It is essential for deeper understanding of composites sensitivity because the combinations of various materials are characterized by different reinforcement ratio; different manufacturing techniques result also in various ranges of the fibers into the composite specimen. The results obtained above are valid for 50% reinforcement into the composites RVE and can change for even small variations of the fiber to matrix volumetric ratio.

Computational homogenization methodology implemented in the program MCCEFF needs some further improvements especially towards error analysis and, therefore, mesh adaptation procedures [13]. It is important since large stress gradients are obtained in the finite elements along the interface, where stress boundary conditions are applied. The effective elasticity tensor must be well-preserved from these inaccuracies (being a single numerical error source) in further simulations.

Finally, let us note that this methodology can be extended on thermoelastic analysis [3], to include some interface defects among the components, towards the multicomponent composites homogenization, as well as on the case study, where statistical description of initial material parameters is also included in the computational procedure.

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