On upper and lower limits of elastic coefficients of SMC composite materials

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Abstract: - The aim of the paper is to present an original homogenization method for elliptic equations applied to pre-impregnated composite materials, known as prepregs. In this class of prepregs can be included Sheet- and Bulk Molding Compounds. Sheet Molding Compounds (SMC) are characterized, in general, as multiphase heterogeneous and anisotropic composite materials with randomly discontinuous reinforcement. The upper and lower limits of the homogenized coefficients for a 27% fiber volume fraction SMC are computed. It is presented a comparison between the upper and lower limits of the homogenized elastic coefficients of a SMC material and the experimental data. The computing model used as a homogenization method of these heterogeneous composite materials, gave emphasis to a good agreement between this method and experimental data.

Key-Words: - Sheet Molding Compounds, Bulk Molding Compounds, Prepregs, Homogenization, Heterogeneity, Computing model, Elliptic equations, Elastic coefficients, Roving.

1 Introduction

Theoretical researches regarding the behaviour of heterogeneous materials lead to the elaboration of some homogenization methods that try to replace a heterogeneous material with a homogeneous one. The aim is to obtain a computing model which takes into account the microstructure or the local heterogeneity of a material.

The homogenization theory is a computing method to study the differential operators convergence with periodic coefficients. This method is indicated in the study of media with periodic structure. The most obvious mechanical model which reflects this model is a Sheet Molding Compound (SMC) material. A SMC is a pre-impregnated composite material, known as prepreg, chemically thickened, manufactured as a continuous mat of chopped glass fibers, resin (known as matrix), filler and additives, from which blanks can be cut and placed into a press for hot press molding. The result of this combination of chemical compounds is a heterogeneous, anisotropic composite material reinforced with randomly disposed discontinuous reinforcement [1], [2], [3].

The matrix- and fillers elastic coefficients are very different but periodical in spatial variables. This periodicity or frequency is suitable to apply the homogenization theory to the study of heterogeneous materials like SMCs.

2 Problem formulation

Let us consider Ω a domain from R^3 space, in coordinates x_i, domain considered a SMC composite material, in which a so called substitute matrix (resin and filler) is represented by the field Y_1 and the reinforcement occupies the field Y_2 seen as a bundle of glass fibers, (fig. 1).

Let us consider the following equation [4]:

$$f(x) = -\frac{\partial}{\partial x_i}\left[a_{ij}(x)\cdot\frac{\partial u}{\partial x_j}\right];\quad a_{ij} = a_{ji}, \tag{1}$$

or under the equivalent form:

$$f = -\frac{\partial p_i}{\partial x_i};\quad p_i = a_{ij}\cdot\frac{\partial u}{\partial x_j}. \tag{2}$$

In the case of SMC materials that present a periodic structure containing inclusions, $a_{ij}(x)$ is a function of x. If the period's dimensions are small in comparison with the dimensions of the whole domain then the solution u of the equation (1) can be considered equal with the solution suitable for a homogenized material, where the coefficients a_{ij} are constants.

In the R^3 space of y_i coordinates, a parallelepiped with y_i^0 sides (fig. 1) is considered, as well as parallelepipeds obtained by translation $n_i y_i^0$ (n_i integer) in axes directions.

The functions:

$$a_{ij}^{\eta}(x)=a_{ij}\left(\frac{x}{\eta}\right), \qquad (3)$$

can be defined, where η is a real, positive parameter. Notice that the functions $a_{ij}(x)$ are ηY-periodical in variable x (ηY being the parallelepiped with ηy_i^0 sides).

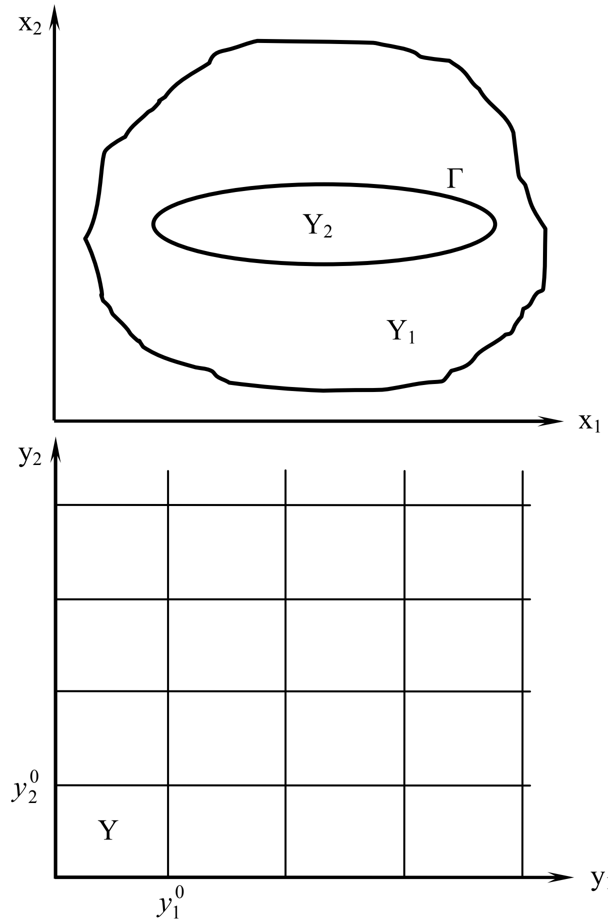

Fig. 1. Domains- and inclusions' periodicity definition of SMC composite materials [4]

If the function $f(x)$ is in Ω defined, the problem at limit can be considered:

$$f(x)=-\frac{\partial}{\partial x_i}\left[a_{ij}^{\eta}(x)\cdot\frac{\partial u^{\eta}}{\partial x_j}\right], \qquad (4)$$
$$u^{\eta}\big|_{\partial\Omega}=0.$$

Similar with equation (2), the vector $\vec{p}^{\eta}$ can be defined with the elements:

$$p_i^{\eta}(x)=a_{ij}^{\eta}(x)\cdot\frac{\partial u^{\eta}}{\partial x_j}. \qquad (5)$$

For the function $u^{\eta}(x)$ an asymptotic development will be looking for, under the form:

$$u^{\eta}(x)=u^0(x,y)+\eta^1u^1(x,y)+\eta^2u^2(x,y)+\ldots;\ y=\frac{x}{\eta}, \qquad (6)$$

where $u^i(x,y)$ are Y-periodical in y variable. The functions $u^i(x,y)$ are defined on Ω x R^3 so that the derivatives behave in the following manner:

$$\frac{d}{dx_i}\rightarrow\frac{\partial}{\partial x_i}+\frac{1}{\eta}\cdot\frac{\partial}{\partial y_i}. \qquad (7)$$

If the values of $u^i\left(x,\frac{x}{\eta}\right)$ are compared in two homologous points P_1 and P_2, homologous through periodicity in neighbour periods, it can be notice that the dependence in $\frac{x}{\eta}$ is the same and the dependence in x is almost the same since the distance P_1P_2 is small (fig. 2). Let us consider P_3 a point homologous to P_1 through periodicity, situated far from P_1. The dependence of u^i in y is the same but the dependence in x is very different since P_1 and P_3 are far away. For instance, in the case of two points P_1 and P_4 situated in the same period, the dependence in x is almost the same since P_1 and P_4 are very close, but the dependence in y is very different since P_1 and P_4 are not homologous through periodicity. The function u^{η} depends on the periodic coefficients a_{ij}, on the function $f(x)$ and on the boundary $\partial\Omega$. The development (6) is valid at the inner of the boundary $\partial\Omega$, where the periodic phenomena are prevalent but near and on the boundary, the non-periodic phenomena prevail [5], [6], [7], [8], [9].

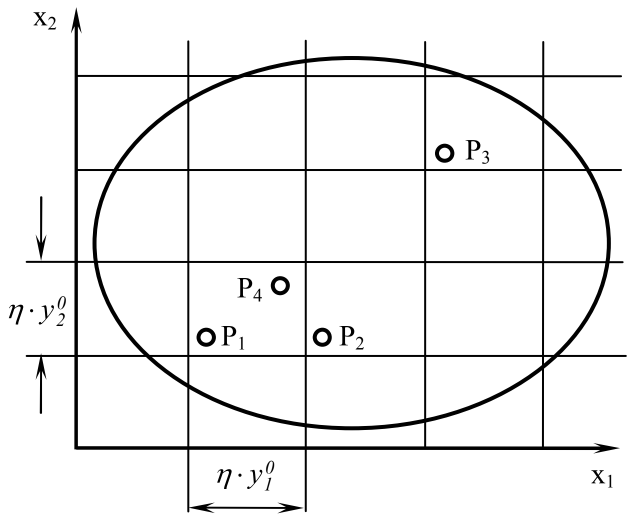

Fig. 2. Physical meaning of SMCs inclusions' periodicity [4]

Using the development (6), the expressions $\frac{\partial u^{\eta}}{\partial x_i}$ and p^{η} can be computed as following:

$$\frac{\partial u^\eta}{\partial x_i} = \left(\frac{\partial}{\partial x_i} + \frac{1}{\eta}\cdot\frac{\partial}{\partial y_i}\right)\cdot\left(u^0 + \eta\cdot u^1 + \ldots\right) =$$

$$= \frac{\partial u^0}{\partial x_i} + \frac{\partial u^1}{\partial y_i} + \eta\cdot\left(\frac{\partial u^1}{\partial x_i} + \frac{\partial u^2}{\partial y_i}\right) + \ldots, \qquad (8)$$

$$p_i^\eta(x) = p_i^0(x,y) + \eta\cdot p_i^1(x,y) + \eta\cdot p_i^2(x,y) + \ldots, \qquad (9)$$

where:

$$p_i^0(x,y) = a_{ij}(y)\cdot\left(\frac{\partial u^0}{\partial x_j} + \frac{\partial u^1}{\partial y_j}\right),$$
$$p_i^1(x,y) = a_{ij}(y)\cdot\left(\frac{\partial u^1}{\partial x_j} + \frac{\partial u^2}{\partial y_j}\right), \ldots \qquad (10)$$

The function $f(x)$ presented in equation (4) can be written in the following manner:

$$f(x) = \left(-\frac{\partial}{\partial x_i} - \frac{1}{\eta}\cdot\frac{\partial}{\partial y_i}\right)\cdot\left(p_i^0 + \eta\cdot p_i^1 + \ldots\right). \qquad (11)$$

The terms η^{-1} and η^0 will be:

$$\frac{\partial p_i^0}{\partial y_i} = 0, \qquad (12)$$

$$f(x) = -\frac{\partial p_i^0}{\partial x_i} - \frac{\partial p_i^1}{\partial y_i}. \qquad (13)$$

Equation (13) leads to the homogenized- or macroscopic equation. For this, we introduce the medium operator defined for any function $\Psi(y)$, Y-periodical:

$$\langle\Psi\rangle = \frac{1}{|Y|}\int_Y \Psi(y)dy, \qquad (14)$$

where $|Y|$ represents the periodicity cell volume. To obtain the homogenized equation, the operator (14) is applied to the equation (13):

$$f(x) = -\frac{\partial\langle P_I^0\rangle}{\partial x_i} - \left\langle\frac{\partial p_i^1}{\partial y_i}\right\rangle. \qquad (15)$$

According to the operator (14), the second term of the left side of the equation (15) becomes:

$$\left\langle\frac{\partial p_i^1}{\partial y_i}\right\rangle = \frac{1}{|Y|}\int_Y \frac{\partial p_i^1}{\partial y_i}dy = \frac{1}{|Y|}\int_{\partial Y} p_i^1 n_i ds = 0. \qquad (16)$$

Due to Y-periodicity of p_i^1 and the fact that $\vec{n}$ is the normal vector at the boundary of Y, the relation (16) is equal with zero. So, the equation (15) becomes:

$$f(x) = -\frac{\partial\langle P_I^0\rangle}{\partial x_i}. \qquad (17)$$

With help of relation (10), the equation (12) can be written as follows:

$$\frac{\partial}{\partial y_i} = \left[a_{ij}(y)\cdot\left(\frac{\partial u^0}{\partial x_j} + \frac{\partial u^1}{\partial y_j}\right)\right] = 0, \qquad (18)$$

therefore:

$$-\frac{\partial}{\partial y_i} = \left[a_{ij}(y)\cdot\frac{\partial u^1}{\partial y_j}\right] = \frac{\partial u^0}{\partial y_j}\cdot\frac{\partial a_{ij}}{\partial y_j}. \qquad (19)$$

The solution $u^1(y)$ of equation (19) is Y-periodical and to determine it is necessary to introduce the space $U_y(Y) = \{u \in H^1(Y), uY - periodical\}$. The equation (19) is equivalent with the problem to find the solution $u^1 \in U_y$ that verifies:

$$\int_Y a_{ij}(y)\frac{\partial u^1}{\partial y_j}\cdot\frac{\partial v}{\partial y_i}dy = \frac{\partial u^0}{\partial x_j}\int_Y \frac{\partial a_{ij}}{\partial y_i} v dy, \qquad (20)$$

for $\forall v \in U_y$. If $\chi^k \in U_y$ is introduced, with $\langle\chi^k\rangle = 0$, that satisfy:

$$\int_Y a_{ij}(y)\frac{\partial \chi^k}{\partial y_j}\cdot\frac{\partial v}{\partial y_i}dy = \int \frac{\partial a_{ik}}{\partial y_i} v dy, \qquad (21)$$

for $\forall v \in U_y$, then from the linearity of problem (20), its solution can be written under the form:

$$u^1(x,y) = \frac{\partial u^0}{\partial x_k}\chi^k(y) + c(x), \qquad (22)$$

where $c(x)$ is a constant as a function of x. Knowing the expression of u^1 as a function of u^0, from the expressions (10) with (22), the homogenized coefficients can be computed:

$$p_i^0(x,y) = a_{ij}(y)\left(\frac{\partial u^0}{\partial x_j} + \frac{\partial u^1}{\partial y_j}\right) =$$
$$a_{ij}(y)\left(\frac{\partial u^0}{\partial x_j} + \frac{\partial u^0}{\partial x_k}\cdot\frac{\partial \chi^k}{\partial y_j}\right) = \qquad (23)$$
$$= \left[a_{ij}(y) + a_{ij}(y)\cdot\frac{\partial \chi^k}{\partial y_j}\right]\frac{\partial u^0}{\partial x_k}.$$

Applying the medium operator (14), the relation (23) can be written:

$$p_i^0(x) = a_{ik}^0\frac{\partial u^0}{\partial x_k}, \qquad (24)$$

$$a_{ik}^0 = \left\langle a_{ik}(y) + a_{ij}(y)\frac{\partial \chi^k}{\partial y_j}\right\rangle =$$
$$\left\langle a_{ij}(y)\cdot\left(\delta_{jk} + \frac{\partial \chi^k}{\partial y_j}\right)\right\rangle = \langle a_{ik}\rangle + \left\langle a_{ij}\frac{\partial \chi^k}{\partial y_j}\right\rangle. \qquad (25)$$

Therefore, the relation (15) becomes an equation in u^0 with constant coefficients:

$$f = -\frac{\partial}{\partial x_i}\left(a_{ik}^0\frac{\partial u^0}{\partial x_k}\right). \qquad (26)$$

For a composite material in which the matrix occupies the domain Y_1 and presents the coefficient a_{ij}^1, and the inclusion occupies the domain Y_2 with the coefficient a_{ij}^2 separated by a surface Γ, the equation (3) must be seen as a distribution.

3 Problem solution for a SMC

In the case of a SMC composite material which behaves, macroscopically, as a homogeneous elastic environment, is important the knowledge of the elastic coefficients. Unfortunately, a precise calculus of the homogenized coefficients can be achieved only in two cases: the unidimensional one and the case in which the matrix- and inclusion coefficients are functions of only one variable. For a SMC material is preferable to estimate these homogenized coefficients between an upper and a lower limit.

Since the fiber volume fraction of common SMCs is 27%, to lighten the calculus, an ellipsoidal inclusion of area 0,27 situated in a square of side 1 is considered. The plane problem will be considered and the homogenized coefficients will be 1 in matrix and 10 in the ellipsoidal inclusion. In fig. 3, the structure's periodicity cell of a SMC composite material is presented, where the fibers bundle is seen as an ellipsoidal inclusion.

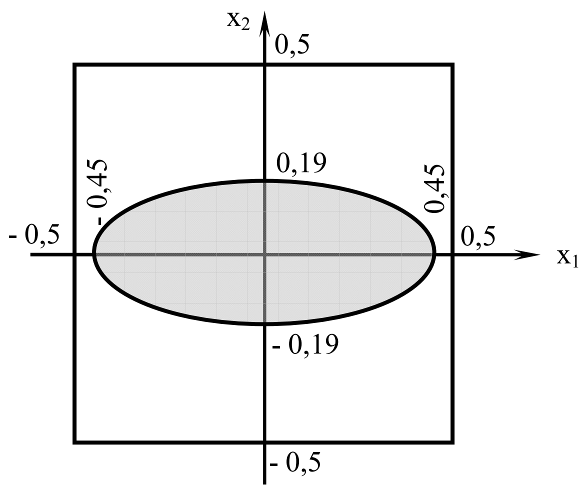

Fig. 3. Structure's periodicity cell of a SMC material with 27% fibers volume fraction

Let us consider the function $f(x_1, x_2) = 10$ in inclusion and 1 in matrix. To determine the upper and the lower limit of the homogenized coefficients, first the arithmetic mean as a function of x_2 followed by the harmonic mean as a function of x_1 must be computed. The lower limit is obtained computing first the harmonic mean as a function of x_1 and then the arithmetic mean as a function of x_2. If we write with $\varphi(x_1)$ the arithmetic mean against x_2 of the function $f(x_1, x_2)$, it follows:

$$\varphi(x_1) = \int_{-0,5}^{0,5} f(x_1, x_2)dx_2 = 1, \quad \text{for} \quad x_1 \in (-0,5;\ -0,45) \cup (0,45;\ 0,5), \tag{27}$$

$$\varphi(x_1) = \int_{-0,5}^{0,5} f(x_1, x_2)dx_2 = 1 + 9,45\sqrt{0,2025 - x_1^2}, \quad \text{for} \quad x_1 \in (-0,45;\ 0,45). \tag{28}$$

The upper limit is obtained computing the harmonic mean of the function $\varphi(x_1)$:

$$a^+ = \frac{1}{\displaystyle\int_{-0,5}^{0,5} \frac{1}{\varphi(x_1)} dx_1} = \frac{1}{\displaystyle\int_{-0,5}^{-0,45} dx_1 + \int_{-0,45}^{0,45} \frac{dx_1}{1 + 9,45\sqrt{0,2025 - x_1^2}} + \int_{0,45}^{0,5} dx_1}. \tag{29}$$

To compute the lower limit, we consider $\psi(x_2)$ the harmonic mean of the function $f(x_1, x_2)$ against x_1:

$$\psi(x_2) = \frac{1}{\displaystyle\int_{-0,5}^{0,5} \frac{1}{f(x_1, x_2)} dx_1} = 1, \quad \text{for} \quad x_2 \in (-0,5;\ -0,19) \cup (0,19;\ 0,5), \tag{30}$$

$$\psi(x_2) = \frac{1}{\displaystyle\int_{-0,5}^{0,5} \frac{1}{f(x_1, x_2)} dx_1} = \frac{1}{1 - 3,42\sqrt{0,0361 - x_2^2}}, \quad \text{for} \quad x_2 \in (-0,19;\ 0,19). \tag{31}$$

The lower limit will be given by the arithmetic mean of the function $\psi(x_2)$:

$$a_- = \int_{-0,5}^{0,5} \psi(x_2)dx_2 = \int_{-0,5}^{-0,19} dx_2 + \int_{-0,19}^{0,19} \frac{dx_2}{1 - 3,42\sqrt{0,0361 - x_2^2}} + \int_{0,19}^{0,5} dx_2. \tag{32}$$

4 Results

Since the ellipsoidal inclusion of the SMC structure may vary angular against the axes center, the upper and lower limits of the homogenized coefficients will vary as a function of the intersection points coordinates of the ellipses, with the axes x_1 and x_2 of the periodicity cell. In table 1, the upper and lower limits of the homogenized coefficients for a SMC material is presented and table 2 shows the basic elasticity properties of the isotropic compounds.

The material's coefficients estimation depends both on the basic elasticity properties of the isotropic compounds and the volume fraction of each compound. If we write P_M, the basic elasticity property of the matrix, P_F and P_f the basic elasticity property of the fibers respective of the filler, φ_M the matrix volume fraction, φ_F and φ_f the fibers-respective the filler volume fraction, then the upper limit of the homogenized coefficients can be estimated computing the arithmetic mean of these basic elasticity properties taking into account the volume fractions of the compounds also:

$$A^+ = \frac{P_M \cdot \varphi_M + P_F \cdot \varphi_F + P_f \cdot \varphi_f}{3}. \tag{33}$$

The lower limit of the homogenized elastic coefficients can be estimated computing the harmonic mean of the basic elasticity properties of the isotropic compounds:

$$A_- = \frac{3}{\frac{1}{P_M \cdot \varphi_M} + \frac{1}{P_F \cdot \varphi_F} + \frac{1}{P_f \cdot \varphi_f}}, \tag{34}$$

where P and A can be the Young modulus respective the shear modulus.

Table 1: Upper and lower limits of the homogenized coefficients for a SMC materials

Angular variation of the ellipsoid inclusion	Upper limit a^+	Lower limit $a\_$
0°	2,52	0,83
± 15°	2,37	0,851
± 30°	2,17	0,886

Table 2: Basic elasticity properties of the isotropic compounds and the volume fractions of the SMC compounds

	Matrix	E-fiber glass	Filler
Young mod. *E* [GPa]	3,52	73	47,8
Shear mod. *G* [GPa]	1,38	27,8	18,1
Volume fraction [%]	28	27	45

The glass fibers represent the basic element of SMC prepreg reinforcement. The quantity and orientation of the rovings determine, in a decisive manner, the subsequent profile of the SMC structure's properties.

There are different grades of SMC prepregs: R-SMC (with randomly oriented reinforcement), D-SMC (with unidirectional orientation of the chopped fibers), C-SMC (with unidirectional oriented continuous fibers) and a combination between R-SMC and C-SMC, known as C/R-SMC.

The following micrographs present the extreme heterogeneity and the layered structure of these materials as well as the glass fibers and fillers distribution. The micrographs show that there are areas between 100…200 μm in which the glass fibers are missing and areas where the fibers distribution is very high.

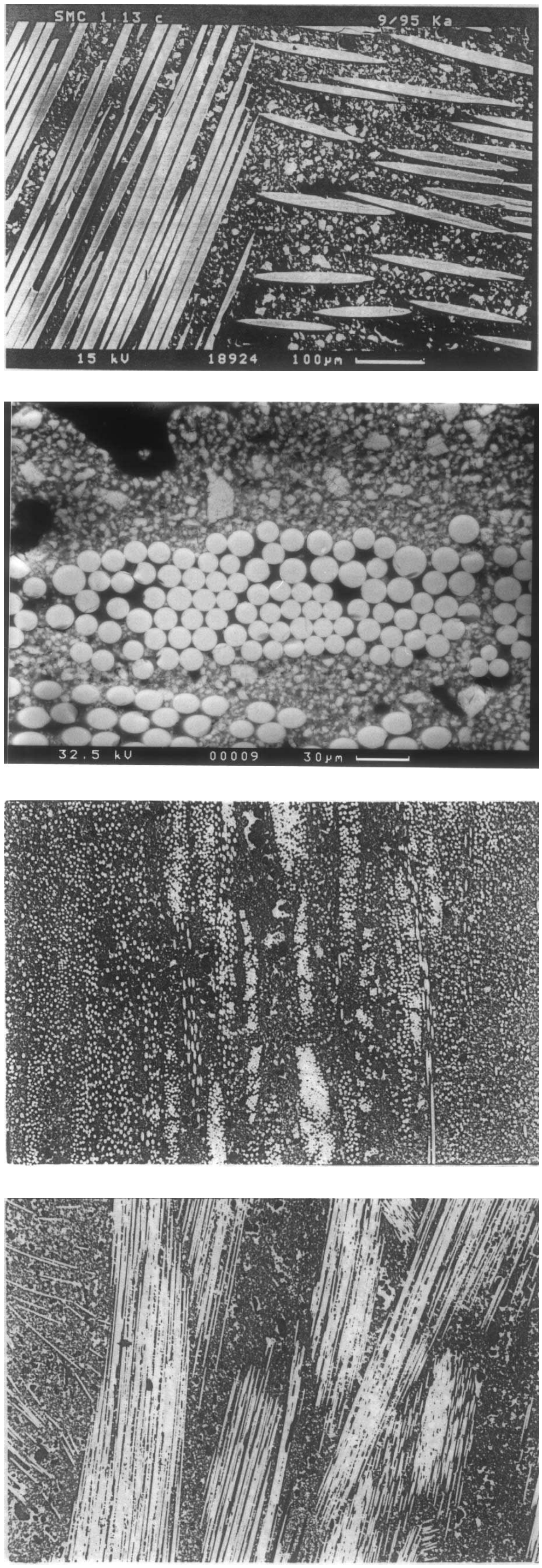

Fig. 4. Micrographs of various SMCs taken in-plane and perpendicular to their thickness [8]

Figure 5 shows the Young moduli and figure 6 presents the shear moduli of the isotropic SMC compounds and the upper and lower limits of the homogenized elastic coefficients.

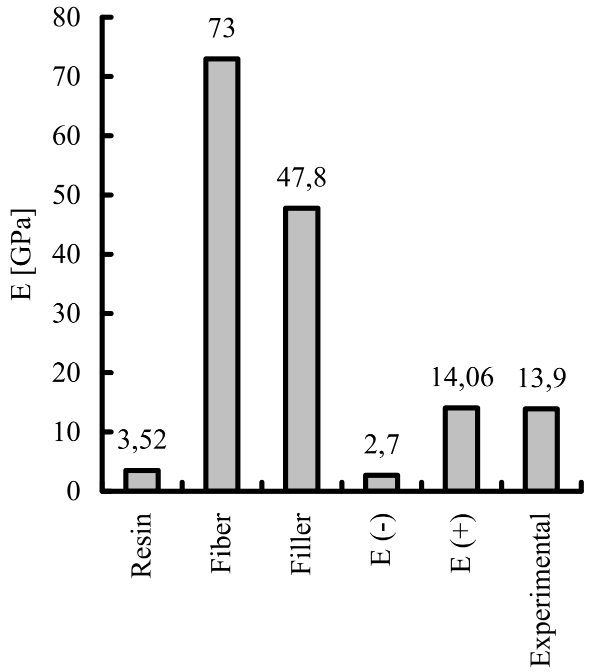

Fig. 5. The values of Young moduli of the isotropic SMC compounds and the upper and lower limits of the homogenized elastic coefficients

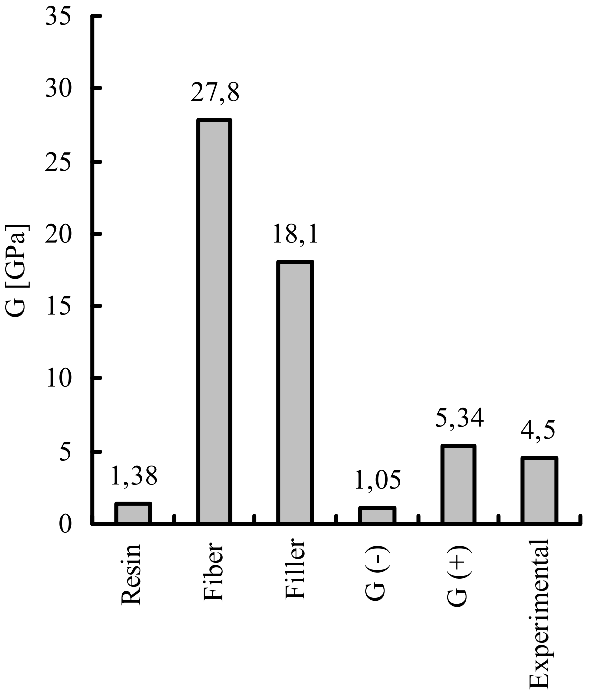

Fig. 6. The values of shear moduli of the isotropic SMC compounds and the upper and lower limits of the homogenized elastic coefficients

5 Conclusions

The presented results suggest that the environmental geometry given through the angular variation of the ellipsoidal domains can leads to different results for the same fibers volume fraction. This fact is due to the extreme heterogeneity and anisotropy of these materials.

The upper limits of the homogenized elastic coefficients are very close to the experimental data.

The proposed estimation of the homogenized elastic coefficients of pre-impregnated composite materials can be extended to determine the elastic properties of any multiphase, heterogeneous and anisotropic composite materials.

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