STUDY OF MICROSTRUCTURE EFFECT ON THE MECHANICAL PROPERTIES OF HETEROGENEOUS MATERIALS BY USING STATISTICAL CONTINUUM THEORY

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Abstract
The strong-contrast version of the statistical continuum theory is used to predict the effective mechanical properties of heterogeneous materials. This approach uses n-point probability functions to account for the shape, orientation and distribution of the fillers within the matrix. For validation, the effective mechanical properties of porous P-311 glass are predicted using the strong-contrast approach, and compared to experimental results and to ones calculated using a strong-contrast differential scheme (DS) model, which is based on Eshelby's theory of inclusion embedded in an equivalent continuum matrix. Further, to demonstrate the effectiveness of the strong-contrast approach in dealing with anisotropic materials, the effective mechanical properties of a macroscopically anisotropic heterogeneous material are predicted and compared to ones calculated using the DS model.

1. Introduction

Material heterogeneities may be due either to different atomic or molecular organization in the same material (semi-crystalline polymer, polycrystals ...etc), or to the presence of different constituents (composite materials). The response of these materials to external excitations depends on their overall effective physical properties. Therefore, many analytical models based on volume fractions of each phase are developed and used to predict the effective properties of heterogeneous materials. However, these models are based on different geometrical

simplifications of the real material's microstructure. The simplest models are the parallel model proposed by Voigt [1] and the series model proposed by Reuss [2]. These two models give, respectively, the upper and lower bounds of effective properties of heterogeneous materials using only the volume fraction of each phase. To take into account the microstructure details, some models use an equivalent microstructure close to the real one [3] or use morphological parameters of inclusions [4]. These models show that the use of more microstructure's informations improve significantly the prediction of the effective properties. However, when the ratio between the intrinsic properties of the materials phases increases (strong-contrast), the difference between the bounds provided by the models mentioned above becomes more important. Other models, based on the Eshelby theory [5], give better predictions of the effective properties. In this approach, an average shape of inclusions is considered to take into account the microstructure morphology. However, these models predict successfully the effective physical properties of heterogeneous materials only when the shape of inclusions is simple (sphere, ellipse, plate and cylinder).

In the present work, a strong-contrast approach based on the statistical continuum theory is used to predict the effective mechanical properties of heterogeneous materials. In this approach, n-point probability functions are used to take into account the shape of the material's constituents, their distribution and their orientation. When the difference between the material individual properties is very large, Torquato [6] proposed a strong-contrast formulation for isotropic and anisotropic media for any space dimension. In the present work, we used this approach to study microstructure effect on the effective mechanical properties of two-phase materials, where the difference between the mechanical properties of the two phases is large (strong-contrast). This study is motivated by a recent development of an analytical approximation of three-point probably functions [7], that can be easily implemented and exploited for the calculation of the effective physical properties of heterogeneous materials. For validation of the statistical approach, the predicted effective mechanical properties of porous P-311 glass are compared to experimental data [8] and to numerical ones using the deferential scheme (DS) model that is based on Eshelby's theory of inclusion embedded in an equivalent continuum matrix [9].

2. Theoretical background

In this section we recall briefly the derivation of the effective stiffness tensor based on the strong-contrast approach and the DS model. For more details, the reader might refer to the work of Torquato [10] and Koutsawa et al. [9].

2.1. Strong-contrast approach

The strong-contrast homogenisation of the mechanical properties of two phase materials is summarized in the following equation [10]:

$$\mathbf{L}^{(q)}:\left(\mathbf{L}_e^{(q)}\right)^{-1}=\frac{\mathbf{I}}{S_1^{(p)}(\boldsymbol{x})}-\int_a\left[\frac{S_2^{(p)}(\boldsymbol{x},\boldsymbol{x}')-S_1^{(p)}(\boldsymbol{x})S_1^{(p)}(\boldsymbol{x}')}{S_1^{(p)}(\boldsymbol{x})S_1^{(p)}(\boldsymbol{x}')}\right]\mathbf{U}^{(q)}(\boldsymbol{x}-\boldsymbol{x}')\,d\boldsymbol{x}'$$
$$-\iint_a\left[\frac{S_3^{(p)}(\boldsymbol{x},\boldsymbol{x}',\boldsymbol{x}'')}{S_1^{(p)}(\boldsymbol{x})S_1^{(p)}(\boldsymbol{x}')}-\frac{S_2^{(p)}(\boldsymbol{x},\boldsymbol{x}')S_2^{(p)}(\boldsymbol{x}',\boldsymbol{x}'')}{S_1^{(p)}(\boldsymbol{x})S_1^{(p)}(\boldsymbol{x}')S_1^{(p)}(\boldsymbol{x}'')}\right]\mathbf{U}^{(q)}(\boldsymbol{x}-\boldsymbol{x}'):\mathbf{U}^{(q)}(\boldsymbol{x}'-\boldsymbol{x}'')d\boldsymbol{x}'d\boldsymbol{x}'' \quad (1)$$
$$-\ldots$$

Where the fourth-order tensor $\mathbf{L}^{(q)}$ is related the mechanical properties of each phase by:

$$\mathbf{L}^{(q)} = \left[dK^{(q)} + 2(d-1)G^{(q)} \right] \left[\frac{K^{(p)} - K^{(q)}}{K^{(p)} + \frac{2(d-1)}{d} G^{(q)}} \mathbf{\Lambda}_{(h)} + \frac{(d+2)G^{(q)}}{d(K^{(q)} + 2G^{(q)})} \frac{G^{(p)} - G^{(q)}}{G^{(p)} + \frac{G^{(q)} \left[d\,K^{(q)}/2 + (d+1)(d-2)\,G^{(q)}/d \right]}{K^{(q)} + 2G^{(q)}}} \mathbf{\Lambda}_{(s)} \right],$$

Further the forth order tensor U in eqution (1) is given by:

$$\mathrm{U}_{ijkl}^{(q)}(\boldsymbol{r}) = \mathrm{L}_{ijmn}^{(q)} : \mathrm{H}_{mnkl}^{(q)}(\boldsymbol{r}) \tag{2}$$

Where the fourth order tensor $\mathrm{H}_{mnkl}^{(q)}$ is given by:

$$\begin{aligned} \mathrm{H}_{ijkl}^{(q)}(r) = \frac{1}{2\Omega \left[dK^{(q)} + 2(d-1)G^{(q)} \right]} \frac{1}{|\boldsymbol{r}|^d} \Big\{ & \alpha^{(q)} \delta_{ij}\delta_{kl} - d\left[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} \right] \\ & - d\alpha^{(q)} \left[\delta_{ij} n_k n_l + \delta_{kl} n_i n_j \right] + \frac{d(d-\alpha^{(q)})}{2} \left[\delta_{ik} n_j n_l + \delta_{il} n_j n_k + \delta_{jk} n_i n_l + \delta_{jl} n_i n_k \right] \\ & + d(d+2)\alpha^{(q)} n_i n_j n_k n_l \Big\} \end{aligned}$$

In equation (1), $S_1^{(p)}(\boldsymbol{x})$, $S_2^{(p)}(\boldsymbol{x}, \boldsymbol{x}')$ and $S_3^{(p)}(\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{x}'')$ represent, respectively, the one, two and the three-point probability functions, that take into account the shape, distribution and orientation of the material phases. The one-point probability function is measured by throwing randomly points within the microstructure. Percentage of points located on each phase gives the one-point probability functions $\left(S_1^{(i)}(\boldsymbol{x}), \mathrm{i} = \mathrm{p}, \mathrm{q} \right)$ of each phase, which also represents the volume fraction $\left(\phi_\mathrm{i} = S_1^{(i)}(\boldsymbol{x}), \mathrm{i} = \mathrm{p}, \mathrm{q} \right)$ of each phase. The two and three-point probability functions capture further details of the material's microstructure, and can be measured by throwing randomly vectors within the microstructure. Since only numerical probabilities can be measured directly from microstructures, then their exploitation to calculate effective properties (1) is made possible by the development of corresponding analytical equations whose parameters can be determined from the measured probabilities, such as the Corson approximation for two-probability functions [11]. For three-point probability function, Mikdam et al. [7] proposed an approximation (3) that can be calculated from two-point probability functions:

$$S_3^{(p)}(\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{x}'') \cong \left(\frac{\overline{\boldsymbol{x}\boldsymbol{x}'}}{\overline{\boldsymbol{x}\boldsymbol{x}'} + \overline{\boldsymbol{x}\boldsymbol{x}''}} S_2^{(p)}(\boldsymbol{x}, \boldsymbol{x}'') + \frac{\overline{\boldsymbol{x}\boldsymbol{x}''}}{\overline{\boldsymbol{x}\boldsymbol{x}'} + \overline{\boldsymbol{x}\boldsymbol{x}''}} S_2^{(p)}(\boldsymbol{x}, \boldsymbol{x}') \right) \frac{S_2^{(p)}(\boldsymbol{x}', \boldsymbol{x}'')}{\phi_\mathrm{p}} \tag{3}$$

where $\overline{xx'}$ and $\overline{xx''}$ are distances, respectively, between the positions x and x', x and x''.

2.2. Differential scheme model

This model is based on the Eshelby solution [5] of the elastic problem of an ellipsoidal inclusion. The differential scheme, usually called in the literature as 'self-consistent' approximation, assumes that a composite can be constructed by a gradual addition of infinitesimal quantities of inclusions. Consider a material composed of two isotropic phases with different mechanical properties. Let $\mathbf{C}^{(q)}$ and $\mathbf{C}^{(p)}$ denote the stiffness tensor of the matrix and inclusions, respectively. The effective tensor $\mathbf{C}^{e}$ of this heterogeneous material using the differential scheme is defined as follows:

$$\begin{cases} \dfrac{d\mathbf{C}^{e}}{d\phi} & = \dfrac{1}{1-\phi}\left(\mathbf{C}^{(p)} - \mathbf{C}^{e}\right) : \mathbf{B} \\ \mathbf{C}^{e}_{\phi=0} & = \mathbf{C}^{(q)} \end{cases} \tag{4}$$

where ϕ is the volume fraction of inclusions and $\mathbf{B}$ is the strain concentration tensor expressed by the following equation:

$$\mathbf{B} = \left[\mathbf{I} + \mathbf{S} : \left(\mathbf{C}^{e}\right)^{-1} : \left(\mathbf{C}^{(p)} - \mathbf{C}^{e}\right)\right]^{-1} \tag{5}$$

where $\mathbf{I}$ is the fourth-order identity tensor and $\mathbf{S}$ is the Eshelby tensor, its expression depends on the matrix material properties and the inclusions shape. Higher-order Taylor series is used to calculate $\mathbf{C}^{e}$ for a given volume fraction of inclusions $\phi = \phi_d$. The procedure to compute $\mathbf{C}^{e}\left(\phi_d\right)$ is given as follows:

$$\begin{cases} \phi_0 & = 0 \\ \mathbf{C}^{e}\left(\phi_0\right) & = \mathbf{C}^{(q)} \end{cases} \tag{6}$$

and for $i \geq 1$

$$\begin{cases} \phi_{i+1} & = \phi_i + h_i \\ \mathbf{C}^{e}\left(\phi_{i+1}\right) & = \sum_{k=0}^{N_i} \mathbf{C}^{e}_{k}\left(h_i\right)^{k} \end{cases} \tag{7}$$

where h_i is the size of the N divided interval $\left[0, \phi_d\right]$, $\mathbf{C}^{e}_{k}$ is the k^{th} Taylor coefficient of the function $\mathbf{C}^{e}\left(\phi_i\right)$ and N_i is the order of the Taylor series truncation. For more details of calculation, the reader can refer to Koutsawa et al. [9]).

3. Results and discussions

The strong-contrast approach is used to predict the effective mechanical properties of a porous material. The results are compared to the ones predicted using the DS model and to the experimental results obtained by Walsh et al. [8] in case of a porous glass, where the bulk and shear moduli of the pure glass are $K^{(g)} = 46.3\,\text{GPa}$ and $G^{(g)} = 30.5\,\text{GPa}$, respectively. The microstructures for different pores concentrations used in the statistical approach calculation are computer-generated (Fig.1). The diameter of inclusions is fixed at 10 pixels and their distribution is homogeneous and random. Note that, for pores volume fractions greater than 0.5, it is not possible to generate microstructures with no-overlapping spherical pores (Fig.1a). Therefore, microstructures with partially overlapping inclusions are computer-generated for volume fractions above 0.5 (Fig.1b).

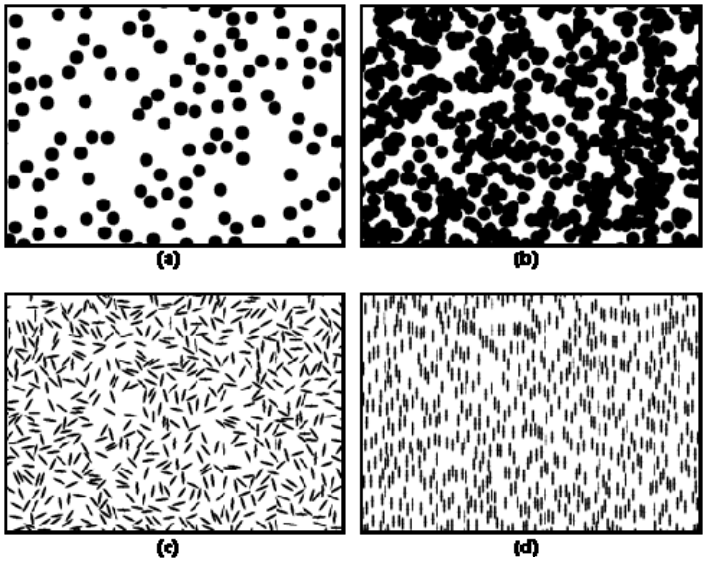

Figure 1. Different microstructures of a material composed of two-phases: phase 1, white part; phase 2, black part. The volume fraction of the phase 2 is 0.2.

Fig.2 shows the predicted effective bulk modulus using the strong-contrast approach versus the pores volume fraction. The mechanical properties of pores are taken zero ($K^{(v)} = 0\,\text{GPa}$ and $G^{(v)} = 0\,\text{GPa}$). Below 0.5 percent of pores concentration, the statistical approach predicted results are slightly lower than the ones predicted using the DS model and the experimental data. However, above the concentration of 0.5 the statistical approach predicts more realistic (closer) effective properties than the DS model. Note that, the improvement of the predict results above the concentration 0.5 using the statistical approach relative to the ones predicted by the DS model is not due to the overlapping pores. Indeed, the effective properties are calculated for overlapping

pores for concentration below 0.5 and the results are found relatively comparable to the ones conducted with no-overlapping pores.

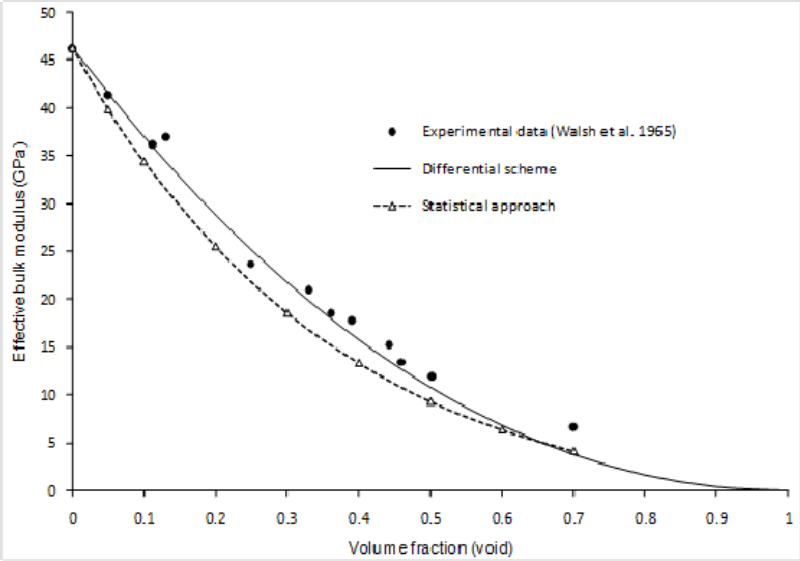

Figure 2. Experimental and numerical effective bulk modulus of porous P-311 glass

To study the effect of orientation and the effectiveness of the statistical approach to take into account the anisotropy, microstructures with oriented (Fig.1d) and non-oriented ellipsoids (Fig.1c) are computer-generated. The semi-major axis is taken equal to 10 pixels and the semi-minor axis equal to 2 pixels. The predicted effective stiffness tensors, in both cases at 0.2 of porosity, using statistical approach are given as follows:

$$\mathbf{C}^{e}_{(\text{non-oriented})} = \begin{pmatrix} 49.53 & 13.55 & 13.39 & 0 & 0 & 0 \\ 13.52 & 49.55 & 13.36 & 0 & 0 & 0 \\ 13.33 & 13.32 & 48.56 & 0 & 0 & 0 \\ 0 & 0 & 0 & 17.81 & 0 & 0 \\ 0 & 0 & 0 & 0 & 17.75 & 0 \\ 0 & 0 & 0 & 0 & 0 & 17.91 \end{pmatrix}$$

$$\mathbf{C}^{e}_{(oriented)} = \begin{pmatrix} 41.09 & 12.67 & 12.41 & 0 & 0 & 0 \\ 12.62 & 41.29 & 12.43 & 0 & 0 & 0 \\ 12.53 & 12.57 & 61.52 & 0 & 0 & 0 \\ 0 & 0 & 0 & 18.06 & 0 & 0 \\ 0 & 0 & 0 & 0 & 18.04 & 0 \\ 0 & 0 & 0 & 0 & 0 & 14.27 \end{pmatrix}$$

Fig.3 shows different coefficients of the stiffness tensor versus porosity in case of oriented ellipsoids. Results obtained using statistical approach are compared to ones predicted by differential scheme. These results have the same form as the one of transversely isotropic materials. It can be seen that the statistical predicted results are in good agreement with the results obtained using differential scheme.

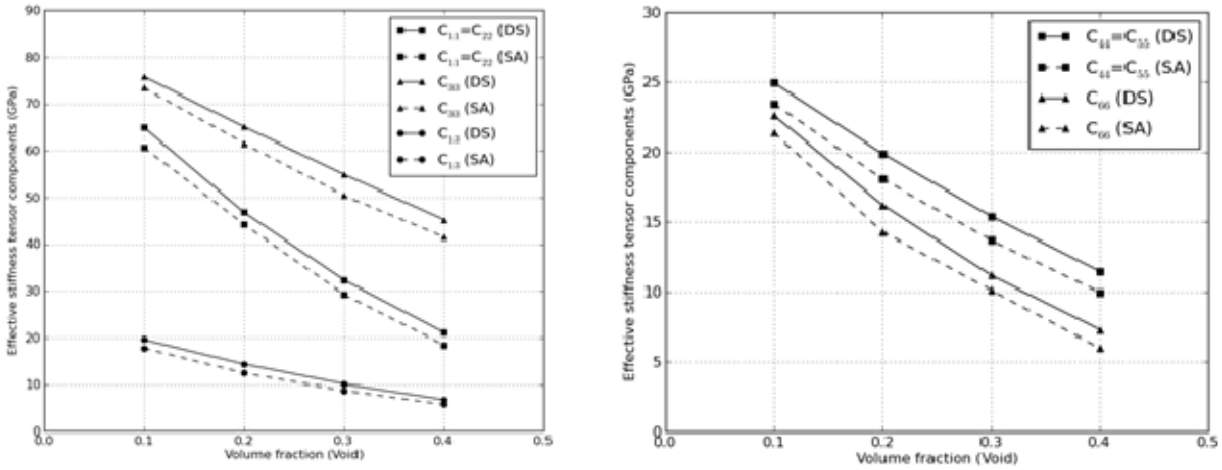

Figure 3: Effective stiffness tensor components (oriented ellipsoids)

4. Conclusions

This paper shows the effectiveness of the statistical continuum theory to predict heterogeneous materials effective properties. Details of the material morphology are taken into account using two-point and three-point probability functions. The strong contrast version (approach) of the statistical continuum theory is implemented and used to calculate the mechanical properties of porous material. The obtained results are compared to experimental data and to ones predicted using the differential scheme model, and a good agreement is found. Further, the effectiveness of the statistical approach in capturing the materials anisotropy is demonstrated by calculation the effective mechanical properties of a heterogeneous material filled with oriented ellipse.

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