Prediction of effective mechanical properties of composite materials using homogenization approach: Application to tungsten fiber reinforced bulk metallic glass matrix composite

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Abstract**—**In this paper, the homogenization approach was presented to predict the effective mechanical properties of heterogeneous materials such as composite materials. Indeed, the main idea of this approach is to characterize the effective mechanical properties from a microstructural description of the heterogeneous materials and the knowledge of the local behavior of constituents using the homogenization process. It is a very efficient tool which is intensively developed in the field of numerical simulation of heterogeneous materials. Different scheme established from the solution of Eshelby's inclusion problem are recalled such as Mori-Tanaka scheme, dilute scheme and Voigt and Reuss bounds. Homogenization approach was applied to estimate the effective mechanical properties of tungsten fiber reinforced bulk metallic glass matrix composite. Predicted values were confronted with those obtained by experimental approach from literature. These comparisons show good agreement between the predicted and experimental values. The maximum deviations remain lower than 10.5% using Voigt bound. A parametric study shows that the mechanical properties depend strongly on the shape of inclusions.

Keywords**—**Composite materials, homogenization method, Eshelby's inclusion problem.

I. Introduction

COMPOSITE materials are increasingly used in several industrial applications such as aerospace, automotive, shipbuilding and offshore oil [1]. Composite materials have high mechanical properties at a low weight. Several approaches based on experience and theoretical models were established to predict the mechanical properties of composite materials. Indeed, the limitations of these approaches have led to the development of the micromechanical approach or multiscale modelling [2, 3]. The main idea of this method is to characterize the macroscopic physical properties from a microstructural description of the heterogeneous material and the knowledge of the local behavior of constituents using the homogenization process [4]. The heterogeneous material is so substituted, through this process, by an equivalent homogeneous material [5]. The explicit analytical expression of equivalent behaviour was established by solving the problem of Eshelby inclusion for simplified geometries [6] (an elastic ellipsoidal inclusion in an infinite elastic matrix). Different solutions have been developed using this approach [7]. In spite of the numerous studies carried out in this field (see for example [8, 9]), the question of the influence of the microstructure on the macroscopic effective properties remains very widely posed. In the last few years, new computational methods were developed to predict the effective properties of composites materials. The most used approaches is based on finite element method [10] and boundary element analysis [11].

In this study, the homogenization approach is used to predict the effective mechanical properties of heterogeneous materials. This method allows to evaluate the influence of microstructure properties on macro behavior of composite materials. A comparison between the experimental values and estimated values was carried on tungsten fiber reinforced bulk metallic glass matrix composite. Indeed, this composite is the subject of widespread research in recent years [12]. It is considered as new generation of structural materials due to their high specific strength, hardness, toughness and corrosion resistance [13-15].

The present study is organized as follows. The basic principles of the homogenization method applied are presented in section 2. The goal is to predict the effective mechanical properties of heterogeneous materials. In section 3, these predictions are confronted with experimental data obtained on tungsten fiber reinforced bulk metallic glass matrix composite. Parametric study highlight the effect of microstructure (shape ratio of ellipsoidal inclusion) on the macroscopic behavior of composite materials. Finally, the major conclusions of the paper are summarized in Section 5.

II. Homogenization approach

The structure of heterogeneous materials can be characterized by three different scales, nanoscopic, microscopic and macroscopic. The last two scales are studied by micromechanics. The macroscopic scale is the real size of the structure. The microscopic scale allows to describe occupied domains of the different phases which consider it as homogeneous. With this scale, we can take into account the phenomena that take place in the material as the interaction

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between the inclusions. At the microscopic level, the material is characterized by d, the size of the heterogeneities and by L, the size of the structure at the macroscopic level. Between these two sizes, it is appropriate to define the size of Representative Volume Element (RVE) of the material, characterized by l. The objective of the homogenization method is to replace a heterogeneous material by an equivalent homogeneous material, such that the laws of macroscopic behavior of two materials are the same. This method is validated if the following both conditions are respected by the three characteristic lengths: $d \ll l$ and $l \ll L$. The first condition is necessary in order to characterize the behavior of RVE by a homogeneous law. The second condition allows to study the structure as a continuous medium. When the conditions of scale separation are verified, a methodology of three successive steps proposed by Zaoui [4] was applied to treat heterogeneous materials. The representation step allows to describe the material at the microscopic scale: description of the phases (shape, spatial distribution...) and definition of the mechanical characteristics of constituents. The localization step allows to determine the relationships between the quantities defined at the microscopic scale and the quantities defined at the macroscopic scale. The homogenization step allows to identify the macroscopic behavior by average operations using the solutions of the localization step.

A. Homogenization of linear elastic media

We are interested in a structure whose constitutive material is linear elastic. The behavior law of this is written as:

$$\begin{cases} \sigma(\underline{x}) = C:\varepsilon(\underline{x}) \\ \varepsilon(\underline{x}) = S:\sigma(\underline{x}) \end{cases} \quad (1)$$

σ: Stress tensor, ε Strain tensor, C: Elasticity tensor and S: Compliance tensor.
The compliance tensor is the inverse of the elasticity tensor:

$$\mathrm{C}:\mathrm{S} = \mathrm{I} \quad (2)$$

With I is the fourth-order identity tensor. Tensors C and S are symmetric tensors, they possesses both minor and major symmetry.

$$\begin{cases} C_{ijkl} = C_{jikl} = C_{ijlk} = C_{jilk} \\ S_{ijkl} = S_{jikl} = S_{ijlk} = S_{jilk} \end{cases} \quad (3)$$

$$\begin{cases} C_{ijkl} = C_{klij} \\ S_{ijkl} = S_{klij} \end{cases} \quad (4)$$

Considering symmetry relations (3) and (4), this results 21 independent components of the elasticity tensor C (or Compliance tensor S).

a- Representation step

First, a microscopic description of the studied structure must be available. To do this, we must identify the phase's number and determine the parameter's nature allowing the description of the corresponding phases. Then, the mechanical behavior of each phase must be characterized. Finally, we must describe the geometry of each phase (the shape, spatial distribution, ...). A RVE occupying the domain Ω of boundary $\partial\Omega$ was considered inside a structure consisting of a heterogeneous linear elastic material. The double condition $d \ll l \ll L$ is satisfied.

b- Localization step

The relations between the microscopic and macroscopic quantities are obtained by the resolution of a problem posed on the domain Ω. Homogeneous boundary conditions are usually used to evaluate overall material properties. A problem was formulated either of homogeneous traction condition or of homogeneous displacement condition imposed on the boundary $\partial\Omega$ of the RVE.

Homogeneous displacement boundary condition

The displacement boundary condition $\underline{u}(\underline{x}) = E.\underline{x}$ is applied on $\partial\Omega$, with E is the macroscopic strain and $\underline{u}(\underline{x})$ is the displacement field at the microscopic scale.
The macroscopic strains E, applied on the boundary of RVE are equal to the spatial average of the local strains in the RVE:

$$\langle\varepsilon\rangle = \frac{1}{|\Omega|}\int_{\Omega} \varepsilon(\underline{x})d\Omega = E \quad (5)$$

The macroscopic stresses Σ are defined by the following relation:

$$\Sigma = \langle\sigma\rangle = \frac{1}{|\Omega|}\int_{\Omega} \sigma(\underline{x})d\Omega \quad (6)$$

For a linear elastic material, the problem to solve at the microscopic scale is then:

$$\begin{cases} \sigma(\underline{x}) = C:\varepsilon(\underline{x}) & (\Omega) \\ div\sigma(\underline{x}) = 0 & (\Omega) \\ \underline{u}(\underline{x}) = E.\underline{x} & (\partial\Omega) \end{cases} \quad (7)$$

The solution of this problem is the microscopic strain field $\varepsilon(\underline{x})$ which is related to macro field E through a still unknown strain concentration tensor A as follows:

$$\varepsilon(\underline{x}) = \mathrm{A}:\mathrm{E} \quad (8)$$

A is a symmetric tensor that checks: $\langle \mathrm{A}\rangle = \mathrm{I}$. In addition, A possesses the minor symmetries ($A_{ijkl} = A_{jikl} = A_{ijlk} = A_{jilk}$) but A does not possesses major symmetries ($A_{ijkl} \neq A_{klij}$).

Homogeneous traction boundary condition

In this case, the traction boundary condition $T = \Sigma.\underline{n}$ is applied on $\partial\Omega$, with Σ is the macroscopic stress and $\underline{n}$ is the surface normal vector. The problem to solve at the microscopic scale is then:

$$\begin{cases} \sigma(\underline{x}) = C:\varepsilon(\underline{x}) & (\Omega) \\ div\sigma(\underline{x}) = 0 & (\Omega) \\ \sigma(\underline{x}).\underline{n}(\underline{x}) = \Sigma.\underline{n}(\underline{x}) & (\partial\Omega) \end{cases} \quad (9)$$

We find that:

$$\sigma(\underline{x}) = \mathrm{B}:\Sigma \quad (10)$$

B is the stress concentration tensor that checks: $\langle B \rangle = I$. In addition, B possesses the minor symmetries ($B_{ijkl} = B_{jikl} = B_{ijlk} = B_{jilk}$) but B does not possesses major symmetries ($B_{ijkl} \neq B_{klij}$).

c- Homogenization step

In this step, the macroscopic behavior will now identify from the previous step.

The Hill-Mandel condition

For any statically admissible stress field and any kinematically admissible strain field, we have the relation:

$$\langle \sigma . \varepsilon \rangle = \Sigma . E \qquad (11)$$

This condition ensures the equality between the macroscopic work ($\Sigma . E$) and the spatial average of the microscopic work ($\langle \sigma . \varepsilon \rangle$).

Homogenization

The homogenized mechanical behavior of RVE can be expressed by linear relationships between the stress and the strain at the macroscopic scale. In the case of the homogeneous strain imposed on the RVE boundary, using the relations (6), (8) and the behavior law (1), this behavior is written in the form:

$$\Sigma = \langle \sigma \rangle = \langle C : \varepsilon \rangle = \langle C : A : E \rangle = \langle C : A \rangle : E = C^{hom} : E \qquad (12)$$

Thus, we obtain a homogenized constitutive law characterized by the homogenized elasticity tensor C^{hom}, with:

$$C^{hom} = \langle C : A \rangle \qquad (13)$$

In the case of the homogeneous traction imposed on the RVE boundary, we show that:

$$E = \langle \varepsilon \rangle = \langle S : \sigma \rangle = \langle S : B : \Sigma \rangle = \langle S : B \rangle : \Sigma = S^{hom} : \Sigma \qquad (14)$$

S^{hom} is the homogenized compliance tensor, with:

$$S^{hom} = \langle S : B \rangle \qquad (15)$$

Tensors C^{hom} and S^{hom} are symmetric tensors (minor and major symmetry). S^{hom} and C^{hom} are not strictly inverses of each other.

B. Eshelby's tensor of the auxiliary linear elastic problems

When In general, the heterogeneous materials such as composites materials contain N phases whose elasticity tensor of each phase is known and homogeneous. The homogenized elasticity tensor C^{hom} of RVE is rewritten as:

$$C^{hom} = \sum_{r=1}^{r=N} \phi_r C_r : A_r \qquad (16)$$

C_r : elasticity tensor of the phase r, A_r : concentration tensor of the phase r, ϕ_r : volume fraction of the phase r.

The determination of the homogenized elasticity tensor C^{hom} is thus reduced to seeking concentration tensors A_r.The expression of A_r can be reached using the famous Eshelby solution [6]. We can consider the auxiliary problem where the inhomogeneity "I" of elasticity tensor C_I is immersed in an infinite homogeneous medium Ω whose elasticity tensor is C_s. The equations of this problem of inhomogeneity are written as follow:

$$\begin{cases} div\, \sigma(\underline{x}) = 0 \\ \sigma(\underline{x}) = C : \varepsilon(\underline{x})\ avec \begin{cases} C = C_I\ for\ \underline{x} \in (I) \\ C = C_s\ for\ \underline{x} \in (\Omega - I) \end{cases} \\ u(\underline{x}) = E . \underline{x}\ when\ (|\underline{x}| \to \infty) \end{cases} \qquad (17)$$

Indeed, these equations define the inclusion problem of Eshelby [6]. The strain field in the ellipsoid domain "I" is written as follow:

$$\varepsilon(\underline{x}) = A_I : E \qquad (18)$$

with :

$$A_I = [I + (C_I - C_s) : P]^{-1}) \qquad (19)$$

P is the Hill's polarization tensor [16].

Hill's polarization tensor

The Hill tensor is a fourth order tensor that depends only on the components of the elasticity tensor of the matrix C_s, the shape and orientation of the inclusions (I). An analytical solution for the polarization tensor was proposed by Withers [17] for transverse isotropic constituent with ellipsoidal heterogeneities. For complementary detail on the tensor of polarization, the reader can refer to the article [17]. Withers [17], Sevostianov et al. [18], Kirilyuk et al. [19] and Giraud et al.[20] have proposed analytical solutions for different shape of heterogeneity (cylinder, sphere, ellipsoid…), in a transversely isotropic media.

C. Some standard schemes for estimating the effective elasticity tensor

The solution of the Eshelby inhomogeneity problem provides an efficient tool to construct different schemes for estimating the effective elasticity tensor. In the following section, the estimation schemes used in this work will be represented.

The Dilute scheme

The dilute scheme stipulates that each inhomogeneity behaves like an isolated heterogeneity in an infinite medium subjected to a uniform temperature gradient field on its boundary, which corresponds to the Eshelby's single heterogeneity problem. The interactions between the inclusions are neglected. The average of the strain filed in inhomogeneity (i) is therefore deduced from the Eshelby's solution:

$$\langle \varepsilon \rangle_i = A_i : E \qquad (20)$$

The average concentration tensor of phase i is given by:

$$A_i = [I + (C_i - C_s) : P_i]^{-1} \qquad (21)$$

C_s : elasticity tensor of the matrix, C_i : elasticity tensor of the phase i (inclusion), P_i : Hill tensor of the phase i.

The estimation of the homogeneous elasticity tensor is obtained by the dilute scheme:

$$C^{dil} = C_s + \sum_{i=2}^{i=N} \phi_i (C_i - C_s) : A_i \qquad (22)$$

The Mori-Tanaka scheme

To take into account the interaction between inclusions (inhomogeneities), another approach often used in the literature, it is the Mori-Tanaka scheme [21]. The main purpose of this scheme is to consider the ellipsoidal inhomogeneity immersed in the infinite homogeneous medium (matrix) subjected to a fictitious strain field. The estimation of the effective elasticity tensor using Mori-Tanaka scheme is expressed by the form:

$$C^{MT} = C_s + \sum_{i=2}^{i=N} \phi_i (C_i - C_s) : A_i : \left[\left(1 - \sum_{i=2}^{i=N} \phi_i\right) I + \sum_{i=2}^{i=N} \phi_i A_i\right]^{-1} \quad (23)$$

Voigt and Reuss bounds

The Voigt bound results from a homogeneous displacement approach, which assumes that the strain is constant in all phases and equal to the imposed macroscopic strain E. Namely in each phase "i": $\varepsilon_i = E$. The strain concentration tensor is reduced everywhere to fourth-order identity tensor $A = I$.

The estimation of the homogeneous elasticity tensor is obtained by the Voigt bound:

$$C^{Voigt} = \sum_{i=1}^{i=N} \phi_i C_i \quad (24)$$

The Reuss bound is the dual approach which considers that the stress is constant in all phases and equal to the imposed macroscopic stress Σ. Namely in each phase "i": $\sigma_i = \Sigma$. The stress concentration tensor is reduced everywhere to fourth-order identity tensor $B = I$.

The estimation of the homogeneous compliance tensor is obtained by the Reuss bound:

$$S^{Reuss} = \sum_{i=1}^{i=N} \phi_i C_i^{-1} \quad (25)$$

The Voigt-bound represents the maximum upper bound whereas the Reuss-bound defines the minimum lower bound of the stiffness.

III. Application of Homogenization Approach

The estimation of effective mechanical properties of composite materials can be achieved using the homogenization approach. Composite taken into account is tungsten fiber reinforced bulk metallic glass matrix composite. The Mechanical properties of tungsten fiber reinforced bulk metallic glass matrix composite are listed in table 1.

	Tungsten fiber (W)	Metallic glass matrix
Young's modulus [GPa]	410	96
Poisson's ratio	0.28	0.36

Table 1 Mechanical properties of tungsten fiber reinforced bulk metallic glass matrix composite

A. Comparison with experimental data

The results obtained by different homogenization schemes presented above have been confronted with experimental Young's modulus data of tungsten fiber reinforced bulk metallic glass matrix composite. For this comparison, experimental results related to this composite material have been performed by Conner et al. [22], Zhang et al. [23], Zhang et al. [24], Zhang et al. [12] and Wang et al. [13]. Variations of the normalized Young's modulus $\frac{E}{E_W}$ (E_W is the Young's modulus of Tungsten fiber) versus the volume fraction of tungsten fiber are illustrated in Fig. 1. This Fig. shows that experimental results are very close to those obtained by the Voigt bound predictions. The difference between experimental measurements and predictions using Voigt bound does not exceed 10.5%. It is to underline that the dilute scheme is only applied to composite materials with a low volume fraction of fiber. However, the Mori-Tanaka scheme remains valid for the inclusions with a volume fraction up to 30% [21].

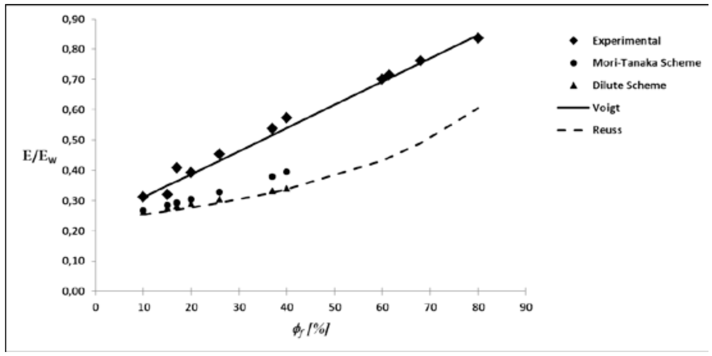

Fig. 1 Variation of the normalized Young's modulus E/E_W (E_W is the Young's modulus of Tungsten fiber) as a function of the volume fraction of tungsten fiber: Comparison between experimental data [12, 13, 22-24] and homogenization schemes.

B. Effect of shape ratio of ellipsoidal inclusion on the effective mechanical properties

In order to study the influence of the microstructure of composite materials, the effect of the shape ratio of the ellipsoidal inclusions on the macroscopic elastic properties is analyzed. The shape ratio w of the ellipsoidal inclusion is defined as :

$$w = \frac{c}{a} \quad (26)$$

a and c are the semi minor axis and semi major axis, respectively, of ellipsoidal inclusions (see Fig. 2)

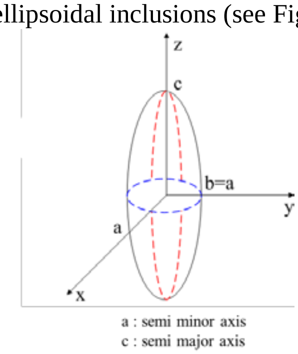

Fig. 2 Ellipsoidal inclusion

The mechanical properties of studied material are calculated according to the fiber volume fraction and for three shape ratios: (see Fig. 3): Oblate ellipsoid inclusion $w = 0.1$, Spherical inclusion $w = 1$ and Prolate ellipsoid inclusion $w = 10$.

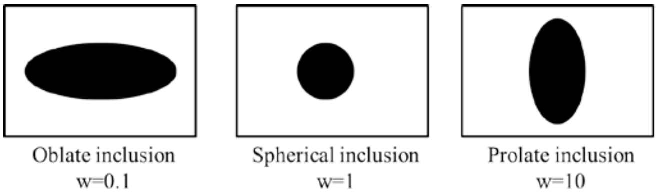

Fig. 3 The three types of ellipsoidal inclusions

The Mori-Tanaka scheme is used to achieve the calculation in this part. Also, the mechanical properties of tungsten fiber and metallic glass matrix are used to estimate the effective mechanical properties for the three types of ellipsoidal inclusions. The main results are summarized on the Fig. 4 and Fig. 5. It is checked that homogenized composite material is transversely isotropic for oblate and prolate inclusions and still isotropic for spherical inclusion. These results underline the effect of the geometry of inclusion on the effective mechanical properties of composite material. For example, for a fiber volume fraction of 20%, the elastic module E_1 vary respectively from 22% for shape ratio $w = 1$ and $w = 10$. Also, for a fixed fiber volume fraction, when the shape ratio of ellipsoidal inclusions increases the Young's modulus E_1 increases and the Young's modulus E_3 decreases.

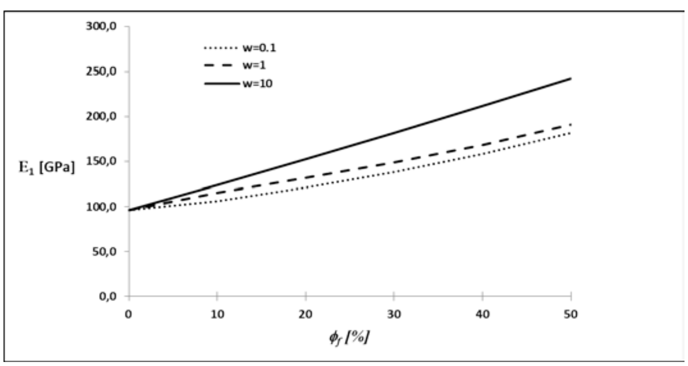

Fig. 4 Modulus E_1 versus the fiber volume fraction for various shape ratios (w =0.1, 1 and 10). Mori-Tanaka scheme

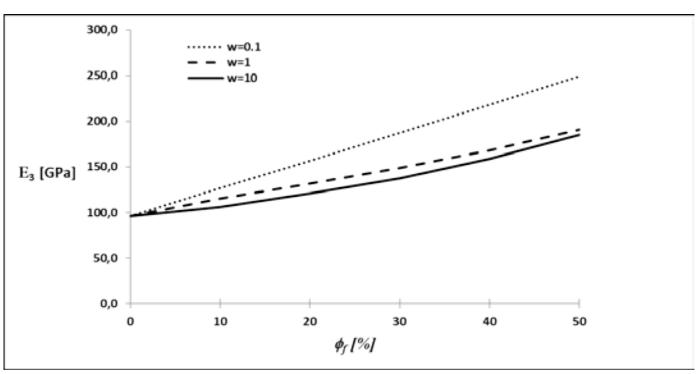

Fig. 5 Modulus E_3 versus the fiber volume fraction for various shape ratios (w =0.1, 1 and 10). Mori-Tanaka scheme

IV. Conclusion

The homogenization approach presented in this paper, proposes a tool for the estimation of effective properties of composite materials. Applied homogenization approach is very efficient from the computational point of view. As an example of homogenization method practical application, the effective mechanical properties of tungsten fiber reinforced bulk metallic glass matrix composite were evaluated and compared with experimental data. A good agreement was observed between the experimental data and the estimated mechanical properties. It is found that the Voigt bound gives the good prediction for studied material. It was shown that the mechanical properties of composite materials depend on the shape ratio of ellipsoidal inclusions. It is reported that the homogenization approach gives only approximate results, therefore detailed stress and strain fields in microstructure cannot be analyzed. In addition, the microstructure's size influence is neglected in homogenization schemes.

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