EVALUATION OF THERMAL EXPANSION OF (AL-SiC) MATERIAL USING HOMOGENEIZATION METHOD COUPLED TO FINITE ELEMENT METHOD

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The determination of the effective properties of a metal matrix composite (MMC) materials seems very important in the characterization, design and manufacturing of composites. The effective coefficient of thermal expansion is among these properties. In this paper a numerical homogenization technique was used to determine the effective coefficient of thermal expansion (CTE). Thus, several 3D numerical models of representative volume elements (RVEs) with different volume fractions have been generated and studied. The influence of spatial distribution and volume fraction of (SiC) particles are examined on the property to study, experimental and analytical estimation were also used to compare their results with those of the numerical method.

Keywords: Coefficient of thermal expansion, Al-SiC composite materials, homogenization, stress

1. Introduction

Metallic matrix composite (MMC) materials are used in several domains of industry because of their relatively simple manufacturing process and almost isotropic properties compared to fiber-reinforced composites, mechanical strength, rigidity, improved creep resistance, and good thermal and electrical conductivity. In particular, aluminum matrix composite materials (AMCs) are used due to their lightness, wear resistance and lower coefficient of thermal expansion [1]. It should be noted here that the method of elaboration of this composite has a great influence on the mechanical and physical properties obtained. Several studies were conducted in an attempt to identify the best combination between the microstructure and the thermo-mechanical properties of MMC with different types of reinforcements, using both particles and fibers [2- 4]. Sharma et al. 2016 [5] have discussed the thermal expansion behavior of densely packed Al-SiC by using a special numerical

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approach, Chawla et al. 2006 [6] have studied the thermal expansion anisotropy in extruded SiC particle reinforced, 2080 aluminum alloy matrix composites, by the use of an experimental thermal mechanical analyzer (TMA) to measure the thermal properties of composites and Finite element method FEM models. Simpler microstructural geometries such as spherical or ellipsoidal shaped particles have been used to model the reinforcement phase distributed in the homogenous matrix, Hua et al. Gu, 2013 [7] and Yin et al. Sun, 2005 [8]. In this work we have considering a model constituted by spherical shaped inclusions of silicon carbide (SiC) embedded in cubic matrix of aluminum (Al) representing a composite microstructure of (Al-SiC) material and we have using an FEM numerical approach to predict the effective coefficient of thermal expansion, the relative expansion behavior and the evolution of the CTE with the temperature change.

2. Generation, meshing and computing of the thermal properties

Concerning the generation of model of composite structure with random sphere, the technique use is random sequential adsorption (RSA) scheme. This technique has been used by several authors, among these authors Moussaddy et al. 2013 [9]; Ghossein et al. 2014 [10]; Boutaani et al. 2017 [11]. The RSA scheme is based on the generation of inclusions with a random distribution, and with the non-overlapping condition of these inclusions.

In order to understand the thermal behavior of the microstructure when it undergoes a change in temperature. We have taking into account 5 sets of representative volume elements (RVEs) with different volume fractions of fillers (5%, 10%, 15%, 20% and 30 %) and we have generated 6 different realizations of volume (number of spheres) (1, 10, 20, 50, 80 and 100) for each volume fraction, using the open-source software BLENDER and PYTHON script [11]. These RVEs composed of spherical inclusions of carbide silicon (SiC) embedded and distributed randomly in a cubic matrix of aluminum (Al), forming (Al-SiC) composite material, and the different configurations are summarized in Table 1.

After generating the models, the commercial FE code COMSOL Multiphysics is used for the evaluation of the coefficient of thermal expansion property and the relative expansion on the volume elements see Fig. 1.

Table 1

Material, volumes (inclusion's number) and volume fraction of inclusions.

Material	Case	Samples	Volume fraction of inclusions
Two -Phase simpler metallic matrix composite (Al-SiC)	Case 1	Contained 01, 10, 20, 50, 80, and 100 spheres of SiC.	5%
	Case 2		10%
	Case 3		15%
	Case 4		20%
	Case 5		30%

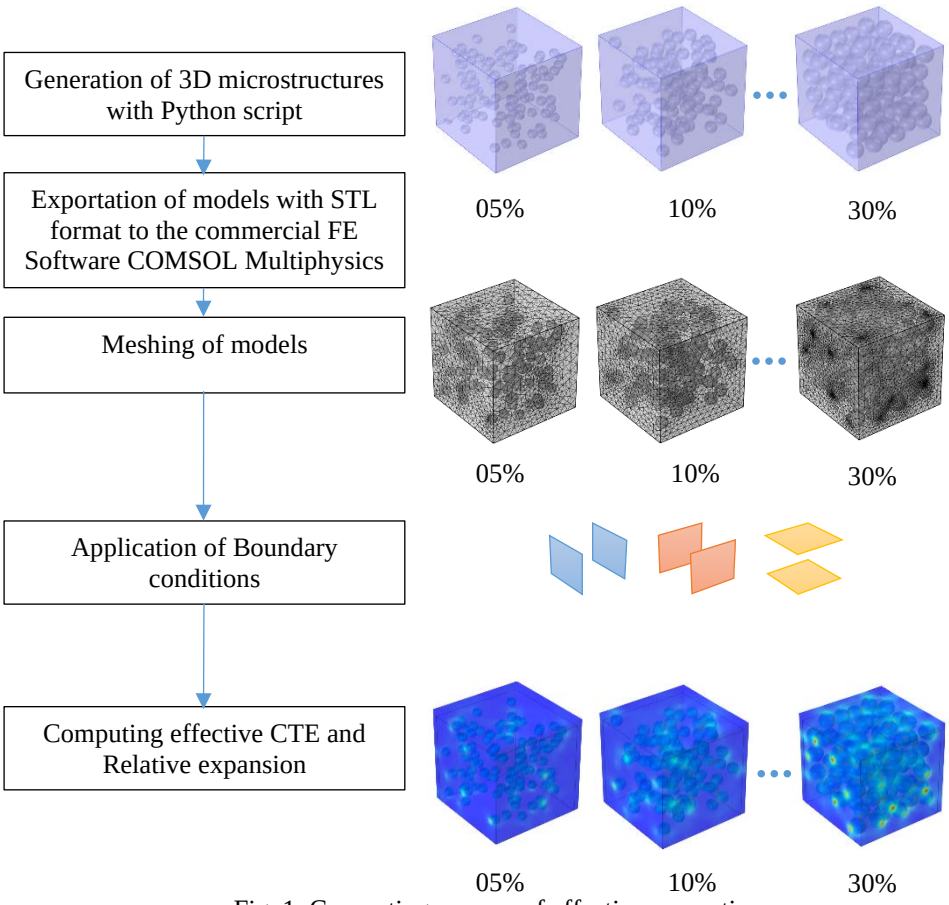

Fig. 1. Computing process of effective properties

2.1. Material and description

We have chosen, a model of microstructure which is constituted of two phases (inclusion and matrix) Fig. 2a. All this represent a representative volume element RVE. This RVE are used to determine the effective coefficient of thermal expansion α^* and the relative expansion.

The temperature-independent properties of constituents of the heterogeneous material, the Young's modulus (E), Poisson ratio (ν) and thermal expansion coefficient (CTE) are given in Table 2.

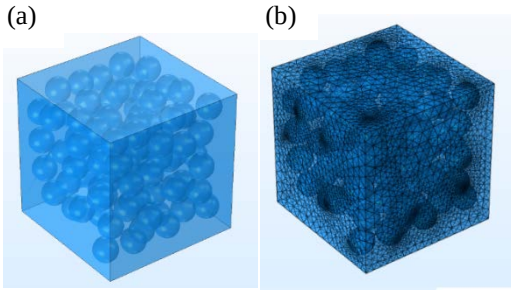

Fig. 2. Examples of microstructures used in this work, (a) 3D cell of microstructure, (b) 3D Mesh

Table 2

Physical properties of composite.

Constituents	E [MPa]	ν [-]	CTE [1/K]
Matrix (Al)	$70X10^3$	0.33	25×10^{-6}
Inclusion (SiC)	400×10^3	0.19	4.3×10^{-6}

2.2. Meshing and Boundary conditions

We introduced meshing considerations for linear static problems. One of the key concepts there was the idea of mesh convergence as you refine the mesh; the solution will become more accurate, but it takes a big study's time and computer's memory. In this paper, the finite element mesh associated with the cell containing spheres, is obtained by the use of free meshing elements see Fig. 2b.

For the convergence, a meshing density of more than 130 000 tetrahedral finite elements was adopted in all this investigation for all simulations Fig. 3.
The homogenization theory is used for the numerical determination of effective thermal expansion properties. A volume element of a heterogeneous material is considered and boundary conditions are prescribed in order to estimate its thermal expansion property.

The boundary conditions are applied on an individual volume element by the use of roller constraints on three planes of the contour ∂V of the RVE ($x = 0$, $y = 0$ and $z = 0$).

All the RVEs are subjected to a temperature change ΔT of 100 K.

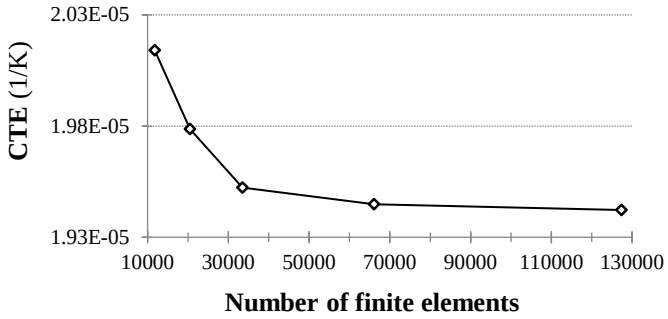

Fig. 3. Convergence of the CTE with respect to mesh density

We define the "apparent coefficient of thermal expansion moduli" (α^{app}) with the analytical expression [12]:

$$\alpha^{app} = \alpha^{*} = \frac{1}{3}\, trace\, \langle \alpha \rangle = \frac{1}{3}\, \langle \alpha_{11} + \alpha_{22} + \alpha_{33} \rangle \tag{1}$$

Where α_{11},α_{22} and α_{33} represent the coefficients of thermal expansion in the 1, 2 and 3 directions, calculated by the numerical method. With the same method and software, we also calculated the relative expansion as

$$\varepsilon = \Delta V / V_0 \tag{2}$$

where ΔV is the volumetric expansion and V_0 is the initial volume.

2.3. Analytical methods to predicting the CTE

There are several analytical methods to predict the coefficient of thermal expansion CTE, among them, the Rule of Mixtures (ROM) is a linear average of the matrix and inclusion's CTE based on volume fraction [10]. The first order equation, Reuss assumption of uniform stress in the composite materials is expressed as:

$$\alpha_c = v_p\, \alpha_p + v_m\, \alpha_m \tag{3}$$

The second equation is The Voigt upper bound [14], the effective thermal expansion coefficient α_c is given by

$$\alpha_c = \frac{v_p E_p \alpha_p + v_m E_m \alpha_m}{v_p E_p + v_m E_m} \tag{4}$$

Where α_p and α_m are the coefficients of thermal expansion of the inclusion and matrix, respectively; v_p, v_m *are* the volume fraction of the inclusion and matrix respectively and E_p, E_m are the Young's modulus of the inclusion and matrix respectively.

Another mathematical model for predicting the CTE of a composite is the Turner model [15]. This model incorporates materials bulk modulus of constituents and expressed as:

$$\alpha_c = \frac{v_p K_p \alpha_p + v_m K_m \alpha_m}{v_p K_p + v_m K_m} \tag{5}$$

where K_p and K_m represent the inclusion and matrix bulk moduli respectively, α_c, α_m, α_p, v_p *and* v_m are the same as from the above method.

The last method is the Schapery model [16]. This model consists of two equations that develop an upper and lower bound for the effective CTE of composites. The upper bound is given by:

$$\alpha_c^u = \alpha_m + \frac{K_p(K_m - K_c^l)(\alpha_p - \alpha_m)}{K_c^l(K_m - K_p)} \tag{6}$$

And lower one as:

$$\alpha_c^l = \alpha_m + \frac{K_p(K_m - K_c^u)(\alpha_p - \alpha_m)}{K_c^u(K_m - K_p)} \tag{7}$$

Where the superscript u and l represent the upper and lower bounds; K_c^u and K_c^l are calculated from the H-S model using the equations below

$$K_c^u = K_p + \frac{v_m}{\frac{1}{K_m - K_p} + \frac{3v_p}{3K_p + 4G_p}} \tag{8}$$

and

$$K_c^l = K_m + \frac{v_p}{\frac{1}{K_p - K_m} + \frac{3v_m}{3K_m + 4G_m}} \tag{9}$$

In the Schapery and H-S equations, all variables are the same as in the previous two models and G_m and G_p represent the shear moduli of the matrix and inclusion, respectively.

3. Results and discussions

In this part, for the evaluation of effective CTE and relative dilation. The numerical simulations based on the finite element method are performed with the periodic boundary conditions.

Before doing the numerical simulation of the effective CTE and the relative expansion of the RVEs, we made assumptions such as, ignoring interface stresses and eventual separation, considering only the elastic properties of the two phases of the composite, no voids in the microstructure. From the results obtained, it appears that there is a homogeneous expansion of the volume in three directions for all the RVEs considered, see Fig. 4.

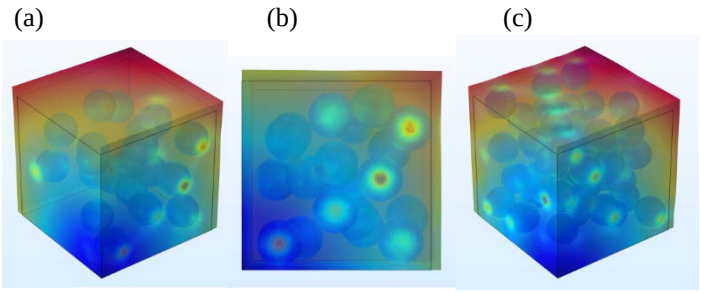

Fig. 4. Expansion of microstructures constituted by: (a) 20 inclusions with 15 % volume fraction in perspective view (b) 20 inclusions and 15 % volume fraction in plane view (b) 50 inclusions with 30% volume fraction in perspective view.

3.1. Effect of volume fraction on the relative expansion

There is a substantial decrease of mean relative expansion with respect to the volume fraction, Fig. 5a. In other hand, there is a very small difference when we change the volume (the number of spheres), so we note negligible effect of the volume (number of spheres) on the relative expansion, see Fig. 6a; this is due to good distribution of the inclusions.

3.2. Effect of volume fraction on the CTE

In Fig. 5b, we take into account the average numerical values of the calculated effective CTEs of each volume fraction and note the evolution of these with respect to the change in the volume fraction of inclusions. The results indicate that the more than the volume fraction of the (SiC) particles is increases, the CTE of (MMC) is decreases. This is due of course, the CTE of the (SiC) is lower than that of the aluminum. It seems to be a negligible difference between the CTEs of the same volume fraction when the volume (number of inclusions) varies, see Fig. 6b. On the other hand, Fig. 7 shows that for volume fractions of 15% (case 3) and 30% (case 5), CTE values vary slightly, due to model errors. Understanding the behavior of thermal expansion helps the designer and manufacturer of metal matrix composite materials to use a proper volume fraction to achieve the desired material.

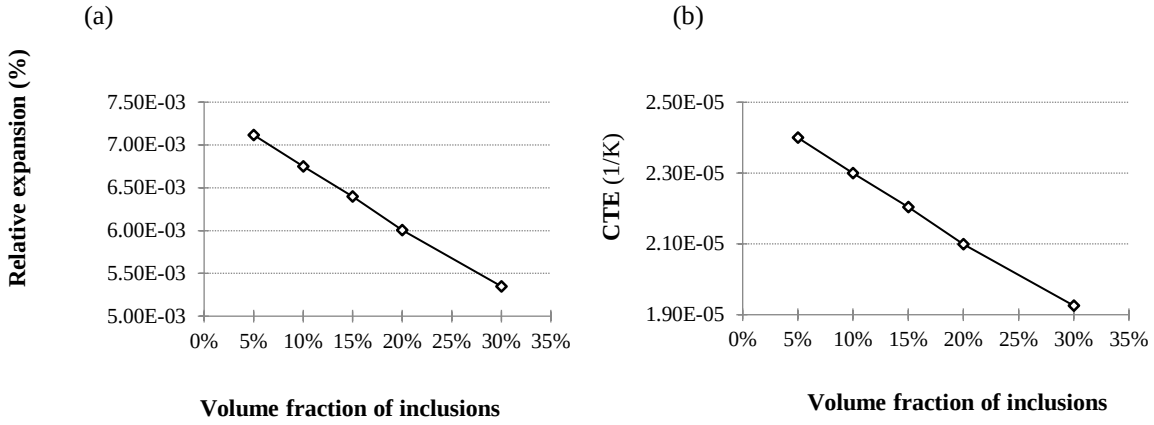

Fig. 5. (a) Relative expansion and mean coefficient of thermal expansion (b) VS. Volume fraction of inclusions

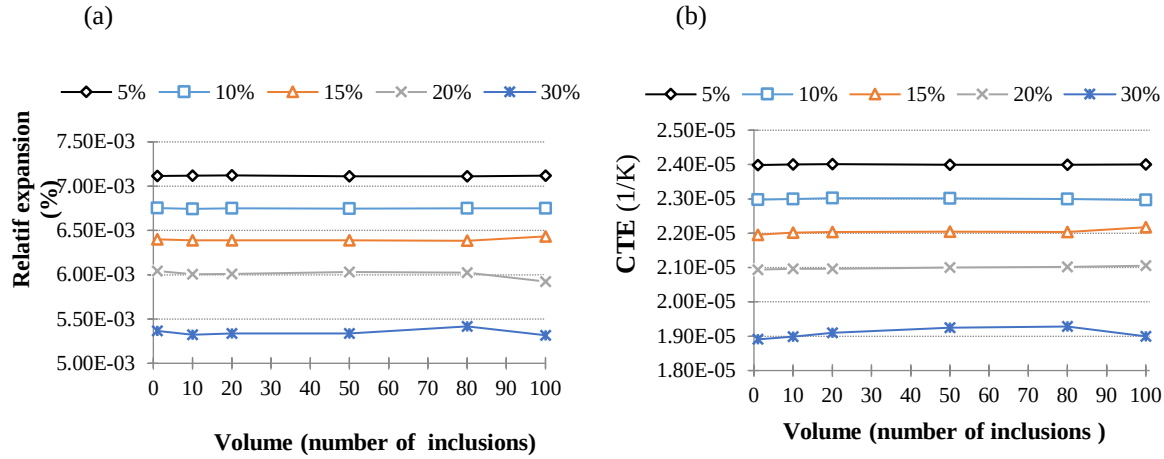

Fig. 6. Effect of volumes (number of inclusions) on: (a) Relative expansions, (b) Effective coefficient of thermal expansion of the microstructures with (5%, 10%, 15%, 20%, 30%) of volume fraction

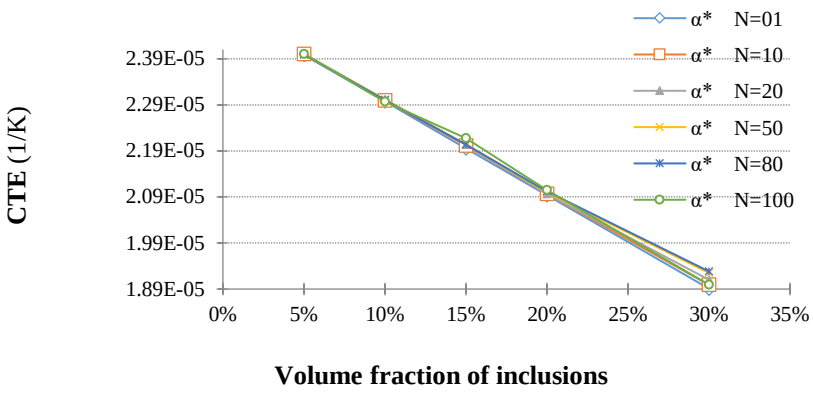

Fig. 7. Effect of Volume fraction of inclusions on the effective coefficient of thermal expansion of microstructures reinforced with N = (01, 10, 20, 50, 80, 100) number of inclusions.

3.3. Effect of temperature on the CTE

We have considered the temperature-dependent properties of the constituents of the material; the data used by [2] and [17], see Table 3. The coefficient of thermal expansion CTE of composite, containing (15%) of SiC, under temperature change (heating from room temperature to 500 °C), is obtained by the FE method and compared to the CTEs obtained by other analytical methods (Sharpy's bounds and Turner's method). To perform that we have taking in consideration several temperatures (50, 100, 200, 300, 400 and 500 °C) the results are illustrated in the Fig. 8.

We note the closer values of effective CTE calculated by the FE numerical method with the values of the Sharpy's upper bound. The relative error between the effective CTE (α*) and the upper bound of Sharpy is taken, because, it is his closest values, should be calculated as:

$$Relative\ error = (\alpha^* - \alpha_{Sh\,U})/\alpha^* \text{x } 100 \tag{10}$$

The resulted values of relative error are acceptable, see Table 4. So, we can deduce that the numerical and the analytical approach of Sharpy upper bound give nearly the same results.

Table 3

The temperature dependence of elastic moduli E (Gpa), Poisson' ratio ν, and CTE (ppm/K) of Al matrix, SiC reinforcement used for the modeling (Huber et Al.2006, Sharma N K et al. 2006)

T(°C)	Al99.5				SiC		
	E [Gpa]	ν	CTE		E	ν	CTE
50	69.2	0.33	22.6		450	0.18	3.8
100	67.6	0.33	24.2		450	0.18	3.8
200	64.0	0.33	25.7		450	0.18	3.9
300	59.8	0.34	27.7		450	0.18	4.0
400	54.9	0.36	30.4		450	0.18	4.0
500	49.9	0.38	31.7		450	0.18	4.1

Table 4

The relative error between the effective CTE α* and the CTE αSh U (upper bound of Sharpy) Versus Temperature

Temperature [°C]	50	100	200	300	400	500
Relative errors [%]	02	04	04	04	04	03

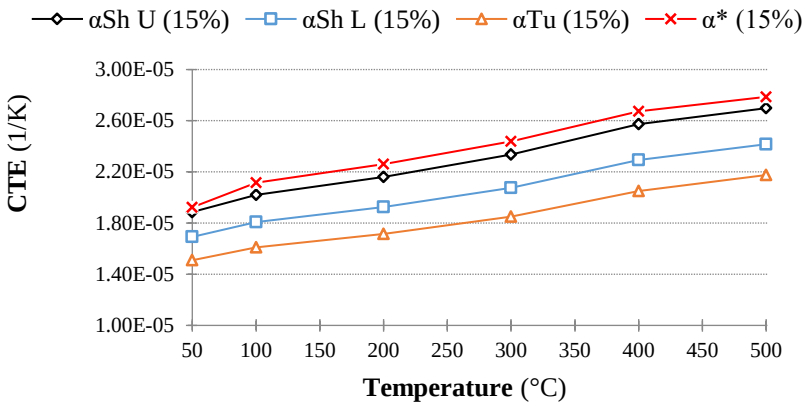

Fig. 8. The effect of temperature change on: Effective coefficient of thermal expansion (α^*), Sharpy's upper (αSh U) and lower bounds (αSh L), and Turner (αTu).

3.4. Effect of the temperature on the residual stress

When the composite material is expanded under the effect of the temperature change, there is an interface stress and deformation between matrix and inclusions. An example of von Mises stress induced on a RVE with (number of spheres 50 and volume fraction 30% of inclusions) is represented in Fig. 9, the interior stresses and deformation between inclusions and matrix may due to the incompatibility of expansion related to the two phases. The stress applied on the inclusions helps to avoiding the separation between the matrix and the fillers at the interfaces. We note here the increase of stresses when the distance between inclusions are very close. And this situation if it is repeated many times (reheating

and cooling) may damage the material. We can distinguish in the Fig. 10, the difference between values of maximum stresses as the volume fraction increase, due to the close distances between inclusions as the volume fraction increase, which causes the increase the difference between stresses of the same volume fraction.

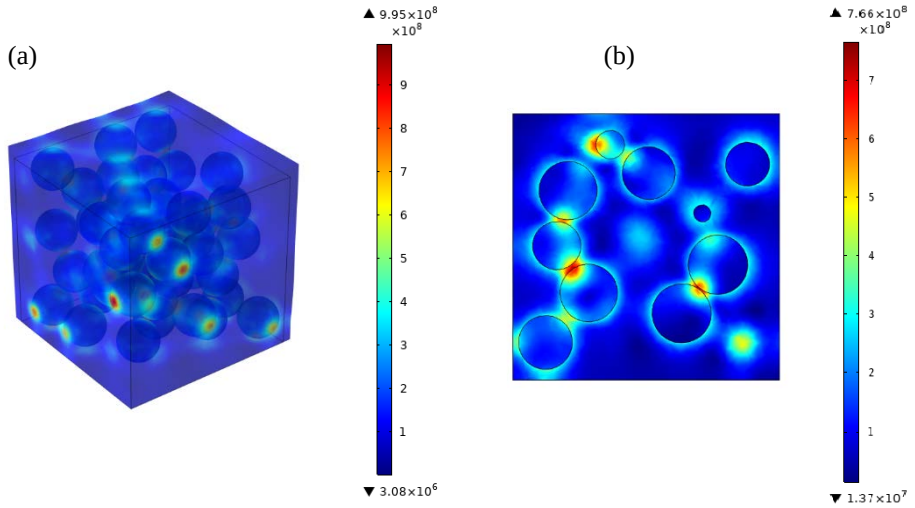

Fig. 9. Von Mises stresses of a RVE with 50 spheres and volume fraction 30%: (a) full view (b) in cross-section view

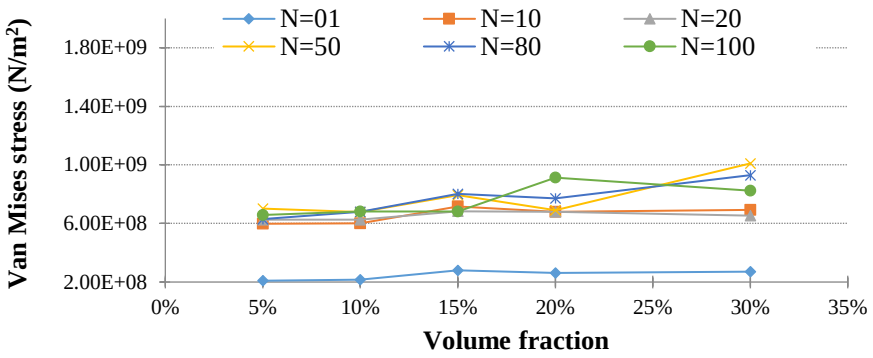

Fig. 10. Von Mises maximum values of stresses in RVEs with different volumes versus volume fractions

3.5. Analytical approaches and FE-approach

In the Fig. 10, we can note that the obtained values of effective CTE calculated by the numerical method is closer to the values of the upper bounds of

Reuss and Sharpy. This allows us the ability to affirm the usefulness of this numerical method to predict the effective coefficient of thermal expansion, in the goal of gaining in time and cost and avoiding destructive controls.

The relative error between the effective CTE (α^*) and the other CTEs (calculated by analytical methods should be calculated as:

$$Relative\ errors = (\alpha^* - \alpha_i)/\ \alpha^* \text{x } 100 \tag{11}$$

When α_i are the analytical calculated values of other CTEs (Reuss, Sharpy, and Voigt). The resulted values of relative errors between α* and the two CTEs of Reuss and Sharpy are acceptable, on the other hand the values of the relative errors between α* and the two CTEs of Turner and Voigt are far from the accepted values, see Table 5.

So, we can deduce that the proposed numerical approach is may be an efficient method to compute the effective CTE of a microstructure.

Table 5

The relative error between the effective CTE α* and the other CTEs Versus volume fraction

Relative errors (%)					
Volume fraction / Analytical methods	5%	10%	15%	20%	30%
α Reuss	0.14	0.31	0.67	0.62	2.42
α Sharpy Upper bound	1.35	2.66	4.10	5.08	8.62
α Sharpy Lower bound	4.37	8.26	11.88	14.73	20.95
α Turner	8.04	14.55	20.03	24.22	31.79
α Voigt	15.77	26.26	33.74	38.91	46.50

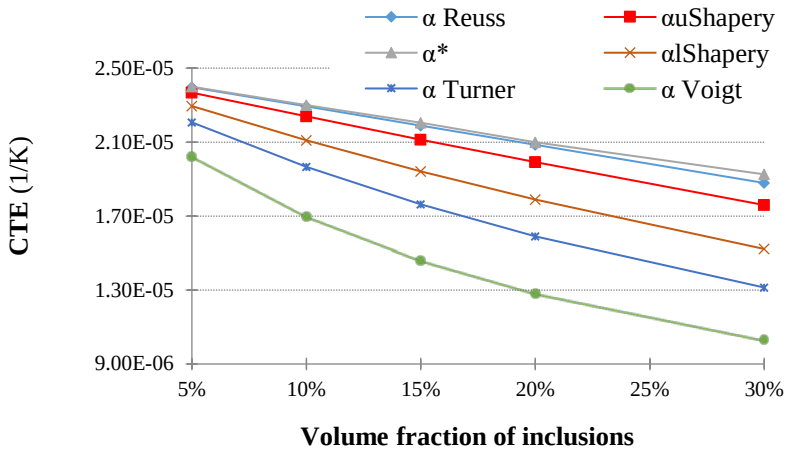

Fig. 10. Comparison between numerical effective CTE calculated with FE-numerical method (α^*) and CTEs calculated by analytical methods.

3.6 Experimental versus numerical methods

The aim work of Chawla et al. 2006 [6] is the study thermal expansion anisotropy of extruded SiC particle reinforced aluminum matrix. Chawla noted that there is a difference in the value of CTE according to the sense of the extrusion process.

The FEM results of the current study, as shown in Fig. 11, show the anisotropy of CTE, which is quite similar to the experimental data. At a particular SiC content (10%), the short transverse direction has the largest CTE followed by transverse and then the longitudinal direction. There is still some difference between the CTE values for the experimental results and those for the FEM results. The main reason for this difference can be attributed to the analysis being carried with a particles of SiC are essentially modeled as irregular forms in the matrix, and in this study all the SiC particles are a spherical one.

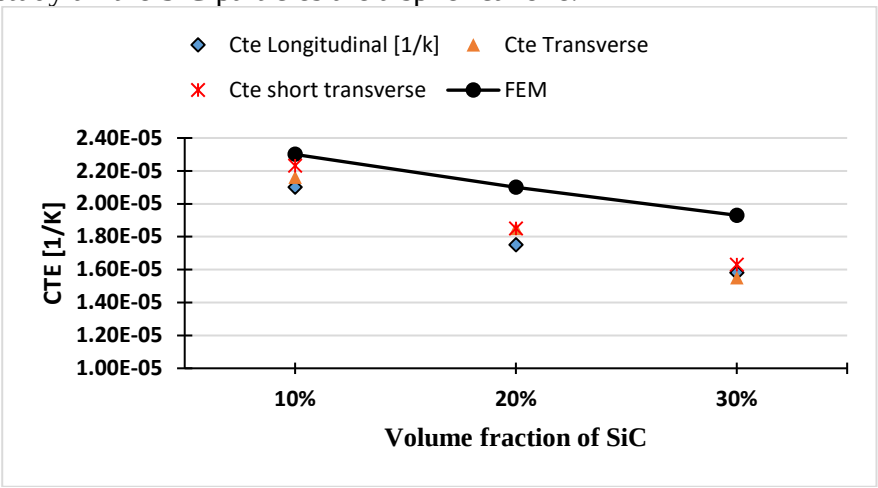

Fig. 11. Comparison between numerical effective CTE with experimental and analytical results CTEs.

4. Conclusion

A 3D numerical models were used to predict the thermal expansion behavior of two-phase composite material precisely (Al/SiC) in the range of mean difference of temperature (20-500 °C) using homogenization techniques for different volume fractions. A numerical method based on the finite element method were used to calculate the effective coefficient of thermal expansion modulus, this one were compared with other CTEs calculated by (Shapery bounds, ROMs bounds, Voigt and Turner) methods and the experimental results.

The numerical results demonstrate that the developed FEM approach is close to some analytical approaches (Reuss and Sharpy's upper bound). The present work indicated that the simpler model of microstructure constituted by a cubic

matrix and spherical spheres is reliable to predict the thermal expansion of the MMCs, and it gives us an acceptable approximation to the desired results.

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