Modelling and Numerical Computation of Thermal Expansion of Aluminium Matrix Composite with Densely Packed SiC Particles

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The coefficient of thermal expansion (CTE) is one of the most important physical properties of metal matrix composites (MMCs). The thermal expansion response is correlated to the microstructure, the deformation of the matrix, and the internal stress conditions. In the present study the physical CTE of aluminium matrix composite (AMC) reinforced with 70 vol. % SiC particles is analytically computed in order to explain abnormalities in the thermal expansion behaviour obtained experimentally. The numerical modelling was carried out from 20^oC to 500^oC using finite element analysis (FEA) based on two-dimensional unit cell models. These unit cell models are created with particular attention on the effects of microscopic voids and phase connectivity obtained from geometrical factors such as the phase shape and particle distribution. The used unit cell models consider the composites as a continuous rigid phase infiltrated with the ductile Al matrix. The obtained thermal expansion behaviour is strongly influenced by the presence of voids. A comparison of physical CTE with the experimental results shows a good agreement.

1 Introduction

MMCs have emerged as a class of materials suitable for advanced structural, electric, thermal management and wear applications. MMCs exhibit significant improvement in physical and mechanical properties compared with unreinforced aluminium alloys, such as in strength, Young's modulus, fatigue resistance, tribological properties and low thermal expansion (Girot et al., 1987; Zweben, 1992; Evans et al., 2003). Aluminium is the most popular matrix for MMCs. The Al alloys are quite attractive due to their low density, their capability to be strengthened by precipitation, their good corrosion resistance, high thermal and electrical conductivity, and their damping capacity. MMCs based on aluminium alloys have received great interest since they combine low weight, high mechanical strength and excellent wear properties, becoming potential as a material for many engineering applications (Evans et al., 2003). AMCs have been widely studied since the 1970s and are now used in sporting goods, electronic packaging, armours and automotive industries, etc. Al alloys reinforced with SiC particles is one of the most suitable and versatile materials among the class of MMCs for use in aerospace and electronic applications, particularly for heat sinks.

Particle reinforced metals (PRMs) with high reinforcement volume fractions (greater than 50 vol.%) are used for thermal management applications such as electronic packaging, partly because of their excellent thermo-physical properties, tailorable thermal expansion response and low density. In general, the thermal expansion behaviour of a composite is the result of several material parameters: the type of constituents and the composites architecture, the reinforcement volume fraction, the internal stresses between the components due to their CTE mismatch, the thermal history, the volume fraction of porosity and the strength of the bonding between the reinforcement and matrix (Huber, 2003a; Huber et al., 2003b, 2006).

MMCs produced by liquid-state processing where the ceramic perform of densely packed particles is infiltrated with molten metal usually exhibit a certain degree of porosity after solidification (Huber et al., 2003b). In the cases where the ceramic content is high, such porosity resulting from incomplete infiltration is expected at the particle contact areas and the sharp concave corners of the ceramic phase. Shen (1997) has shown using finite element analysis that the thermal expansion is strongly influenced by the presence of voids in composites with a continuous ceramic phase. The ceramic can become a continuous phase as a result of specific processing methods employed. The effects of phase connectivity as well as of microscopic voids in the material are expected to play a significant role (Shen, 1997, 1998) with increasing ceramic volume fraction and complementary decrease of metal matrix content.

Numerous experimental studies have been carried out to investigate the CTE of MMCs reinforced with isolated particles (e.g. Frei et al., 2002; Arpón et al., 2003; Zhang et al., 2003a,b). Many theoretical models such as Turner's, Kerner's, and Schapery's have been developed to understand the thermal expansion behaviour of this

kind of MMCs (Yu et al., 2000; Shu and Tu, 2003; Arpón et al., 2003; Zhang et al., 2003a,b, Karadeniz and Kumlutas, 2007). Although these models can be used to predict the dependence of the CTE of PRMs on the reinforcement content, they do not take into account the case for which the reinforcing particles are interconnected or the presence/effects of voids generated during the processing of the composites.

Finite element method (FEM) has been used extensively to simulate the thermal and mechanical behaviour of MMCs. Shen (1997) used the two-dimensional (2-D) unit cell models for numerical modelling of thermal expansion behaviour of MMCs with high reinforcement of volume fractions based on FEA. Recently, Karadeniz and Kumlutas (2007) presented the representative unit cell models to study the effective coefficient of thermal expansion of fibre reinforced composites by micromechanical modelling using the FEM. The results of various finite element solutions for different types of composites were compared with the results of various analytical models and with the available experimental ones. Chawla et al. (2006) presented FEM results using the actual microstructure of Al reinforced with isolated SiC particles to simulate the thermal behaviour. The results showed that the orientation of SiC particles changes the internal stress in the composite yielding on anisotropic thermal behaviour. In general the thermal expansion behaviour of MMCs has been studied numerically based on the micromechanical approach using FEM. Most of the models employ a "unit cell" configuration, where one particle of simple shape is embedded in a continuous metallic matrix shell.

During the present study the unit cell model is applied to analytically determine the influence of voids and interconnectivity of particles on the physical CTE behaviour of an Al matrix composite with high volume fractions of densely packed SiC particles. In a previous experimental study on the CTE (Huber et al., 2006) of Al-based PRMs with 70 vol.% of interconnected and isolated SiC particles, it was proposed that the abnormalities shown by the physical CTE at $T > 250^{\circ}C$ can be explained by filling and re-opening of voids during thermal cycling.

2 Investigated Material and Experimental Results

An AMC reinforced with 70 vol.% of densely packed SiC particles that was produced by gas pressure infiltration of trimodal SiC particles performs (Huber et al., 2006) is investigated. This AMC was investigated in as cast condition. Table 1 lists the designation of the MMC, its matrix composition, the ingredients, fabrication process as well as matrix condition. The microstructure of the AMC is presented in Figure 1.

MMC designation	Matrix	Reinforcement	Fabrication process	Producer	Matrix condition
Al99.5/SiC/70$_p$	Al99.5	SiC$_p$, 70 vol. %, 3-100μm	Gas pressure infiltration	EVAC (Electrovac GmbH, Klosterneuburg, Austria)	As cast

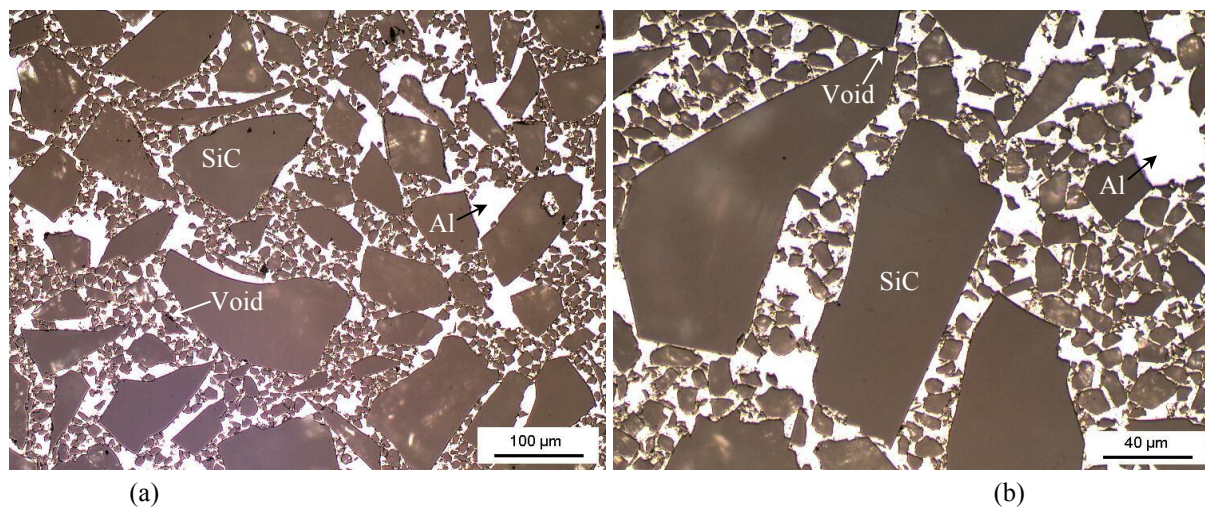Table 1. Overview of the investigated AMC with densely packed SiC particles

Figure 1. Microstructure of investigated material (Al99.5/SiC/70$_p$)

The CTE measurements were carried out from 20°C (RT) to 500°C using a thermo-mechanical analysis equipment (TMA 2940 CE, Thermal Instruments, USA). The specimens were machined into rectangular bars with a size of 4 x 4 x 15 mm^3, the top and the bottom of which were ground and polished to guarantee plane–parallel

surfaces for measurement. The thermal expansion of the samples was measured by a linear position transducer during heating and cooling with rates of 3K/min under nitrogen atmosphere (100ml/min). The specimen temperature was measured using a thermocouple, positioned close to the specimen (Huber, 2003a).

The physical CTE at temperature T is calculated by the following relationship:

$$\text{CTE}(T) = \frac{1}{L}\frac{dL}{dT}$$ (1)

where L is the length of sample as a function of T which was determined from thermal expansion displacement.

Experimentally, the linear expansion with temperature was smoothed in a range of $T \pm 12,5K$ before derivation. Figure 2 shows the temperature dependence of the physical CTEs for the investigated composite (Huber et al., 2006). At lower temperatures up to 200°C the CTEs vary almost linearly with the temperature. A maximum in the CTE curves of the composite could be observed in the range between 200°C to 400°C. Beyond 400°C the composite shows an increase of the physical CTE. Only results from the 2nd thermal cycle will be used for comparison, because the first heating in the experiment starts from an unknown residual stress situation.
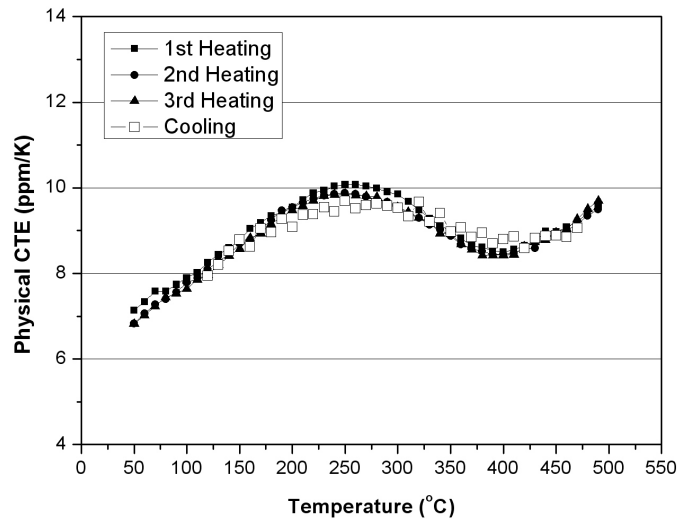
Figure 2. The physical CTEs versus temperature of investigated material (Al99.5/SiC/70$_p$)
for three heating cycles and a cooling cycle representative for the three cycles.

3   Numerical Modelling

In the present work, two unit-cell models that feature a 2-D periodic arrangement of a discretely distributed phase of matrix embedded within 70 vol.% SiC particles as shown in Figure 3 were used. In the case of SiC contiguity, the unit cell model presented by Shen (1997) can be easily achieved by choosing a discrete square-shaped aluminium matrix, as shown in Figure 3a. A SiC network model is shown in Figure 3b. This model represents the small 16 vol. % SiC particles surrounding and contacting with 54 vol.% big particles in the microstructure of the composite. The volume fraction of the bigger particles was measured by quantitative metallography to be 55 ± 2 vol. % (Huber et al., 2003b). Based on the microstructure shown in Figure 1, the model of SiC network shown in Figure 3b is adopted to represent the interconnection between SiC particles. Only one quadrant of the unit cell for both models was used for calculations due to symmetry of the geometry.

The aluminium was considered as a strain hardening elastoplastic solid with temperature dependent material parameters. The SiC particles were treated as isotropic thermo-elastic solids. The properties for all ingredients of the investigated composite used for modelling are listed in Table 2. The plastic response of Al and CTE and Young's modulus as well as Poisson ratio are taken to be function of temperature. The interfaces between Al and SiC as well as SiC particles together were assumed to be perfectly bonded. The volume fraction of voids in modelling was 0.25 vol.%. The boundary conditions are specified taking into account the symmetry of the system. The bottom and left edge of the unit cell quadrant were constrained to have zero displacements in the y and x directions, respectively, while the top and right edge allow for a uniform displacement (symmetry boundary conditions). The expansion displacement at the right and top edges were used to calculate the CTE. A zero stress

condition of all the constituents is chosen for the initial material condition at 20°C. Neither relaxations of Al matrix at elevated temperature nor bonding or debonding at the interfaces are taken into account.
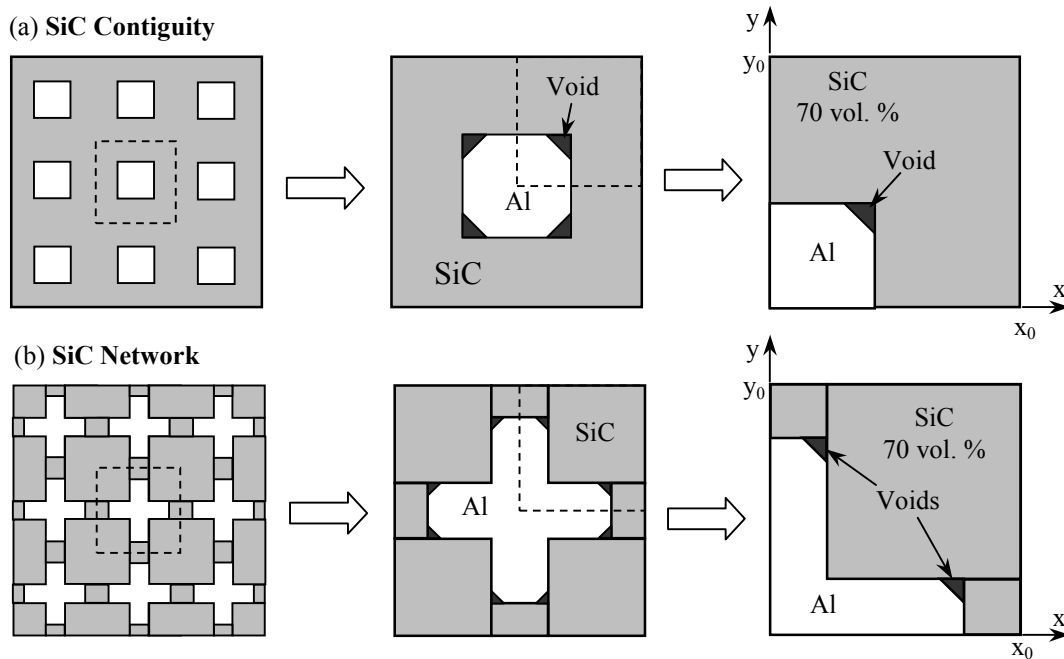

Figure 3. Two-dimensional phase arrangements with microscopic void: unit cell model (a) and (b)

Meshing of unit cells was performed using Altair Hypermesh (Altair Hyperwork), and then imported into the finite element software Abaqus for FEM analysis. A generalized plane strain formulation is used, which is an extension of the plane strain framework. This is done by imposing a constant normal strain perpendicular to the xy-plane on the plane strain state. Although the generalized plane strain model represents fibrous structures extending in z-direction it is applied to the given 2-D arrangement. It gives a more compliant response than the plane stress model, which normally results in a stiffer response than a full three-dimensional analysis (Shen, 1997). The 6-noded triangular elements that were labelled CPEG6 in Abaqus with reduced integration were used for meshing of both the matrix and the reinforcing particles. Unit cell model (a) is meshed using 5766 elements with 11742 nodes as for model (b) using 5390 elements with 11000 nodes. The unit cells were subjected to a uniform temperature change from 20°C to 500°C.

T (°C)	Al99.5				SiC		
	E (GPa)	ν	CTE (ppm/K)	$\sigma_{0,2}$ (MPa)	E (GPa)	ν	CTE (ppm/K)
50	69.2	0.33	22.6	33.0	450	0.18	2.78
100	67.6	0.33	24.2	32.0	450	0.18	3.09
200	64.0	0.33	25.7	24.0	450	0.18	4.16
300	59.8	0.34	27.7	14.5	450	0.18	4.62
400	54.9	0.36	30.4	10.5	450	0.18	4.89
500	49.9	0.38	31.7	9.0	450	0.18	5.09

Table 2. The temperature dependence of elastic moduli E (GPa), Poisson ratio ν, yield stress $\sigma_{0,2}$ (MPa) and CTE (ppm/K) of Al99.5 matrix and SiC reinforcement used for finite element modelling (Huber, 2006; Shen, 1997; King, 1988 and Bauccio, 1994)

4   Numerical Results and Comparison with Experimental Data

The CTE curves during cooling and heating using model (a) with and without void for investigated material are shown in Figure 4. The CTE curves during cooling and heating using model (b) with and without void are shown

in Figure 5. The comparison of CTE curves during heating between the two unit cell models is shown in Figure 6. The relative thermal expansions (RTE) of the composite using model (a) and (b) during the three thermal cycles are shown in Figure 7 and Figure 8, respectively. Commonly three parameters are used to characterize these curves. The first parameter $\Delta\varepsilon^c$ is defined as the largest vertical difference between the heating and cooling curves and is used to quantify the hysteresis of the cycle. The second parameter ε^c, usually referred to as cyclic strain, gives an information equivalent to that provided by the linear CTE obtained from fittings over the whole temperature range. The third parameter ε_r characterizes the residual strain after a thermal cycle. The contour plot of von Mises stress in the Al99.5/SiC/70$_p$ at 500°C during heating using model (b) is observed in Figure 9. It can be observed that the void closes during heating of the composite. Figure 10 shows contour plot of von Mises stress in the whole Al99.5/SiC/70$_p$ at 20°C during cooling using model (b). Here, the void has partially reopened during cooling, but does not reach its original shape. The void closure and re-opening can be observed clearly in Figure 11.

5   Discussions of the Results

The numerical results of physical CTE for the models with void showed a better agreement with the experiments than without void (see Figures 4-6). The CTE of the composite during heating increases almost linearly with the temperature up to 200°C for the investigated models and experiments (region I). In case of the void-containing models the maximum in the CTE curve drops in the transition temperature region (region II) following the experimental results. Figure 9 to Figure 11 showed the void closure and re-opening during heating and cooling. This shows that the drop of CTE in region II of the composites is caused by the filling of voids by plastic deformation of the matrix and confirms the hypothesis proposed by Huber et al. (2006). The increase of maximal Von Mises stress in the SiC bridge from 400 to 500°C amounts to 8.08e+08 MPa (see Figure 11). Von Mises stresses as observed in the SiC particles as well as in the metal matrix are highest close to the SiC particles. In region III the CTE increases again indicating that the void is getting filled producing again elastic straining of the constituents (Huber et al., 2006). The experimental results of the 2nd cycle during heating and cooling are included in Figures 4-6 for comparison. The calculated physical CTE during cooling of both models with void (Figures 4-5) is higher than the experimental one for temperatures down to 300°C. From 300°C down to 200°C both the experimental and calculated results are in good agreement and below 200°C, the modelling results are up to 1ppm/K higher than the experimental ones.

Model (b) with voids showed a good agreement with the experimental results during heating, while model (a) with void showed a difference compared with experimental data. The maximum difference of CTE between the first heating cycle of model (b) and the experiments is less than 1ppm/K which is in the range of the experimental scatter. The largest difference between the heating and cooling $\Delta L/L_o$ curves is quantified by the hysteresis in the thermal strain response as described in (Arpón et al., 2003; Shu and Tu, 2003). The hysteresis parameter of investigated composite using the models with void is indicated in Figure 7 and Figure 8. The decrease in physical CTE values from 250°C to 400°C leads to a residual strain and hysteresis in thermal cycling curves as described by Kumar et al. (2005). The difference in the curves related to cooling may originate from experimental uncertainties but can be explained plausibly by assuming the opening of more pores during cooling than existed before the thermal cycle.
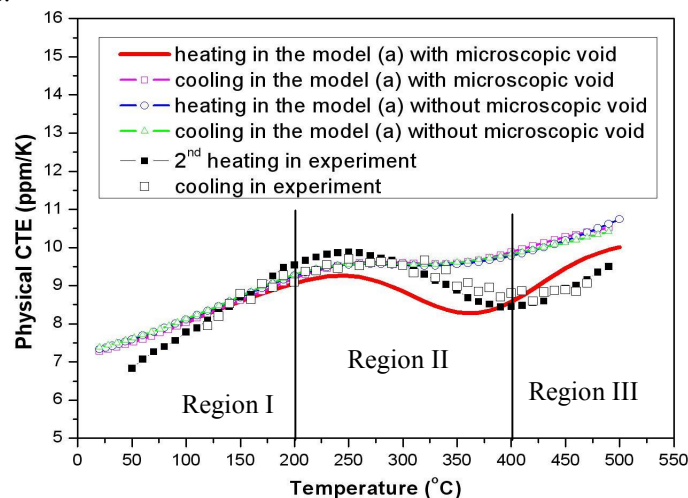

Figure 4. The physical CTEs versus temperature of Al99.5/SiC/70 $_p$ using model (a) with and without void.
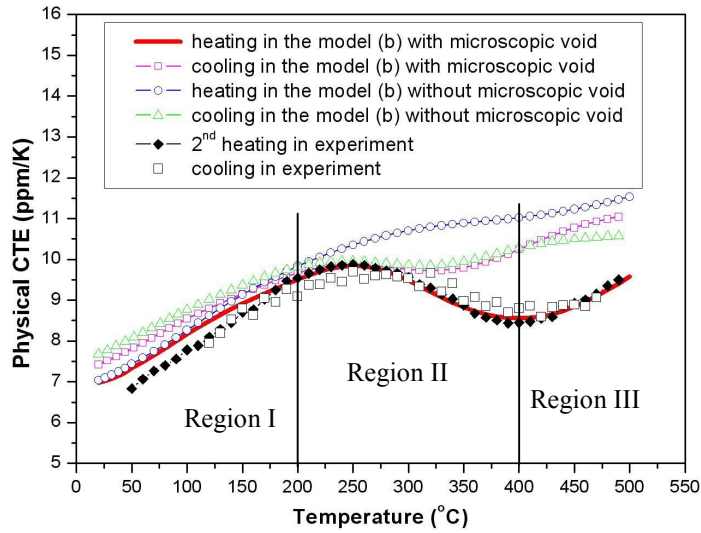
Figure 5. The physical CTEs versus temperature of Al99.5/SiC/70$_p$ using model (b) with and without voids.
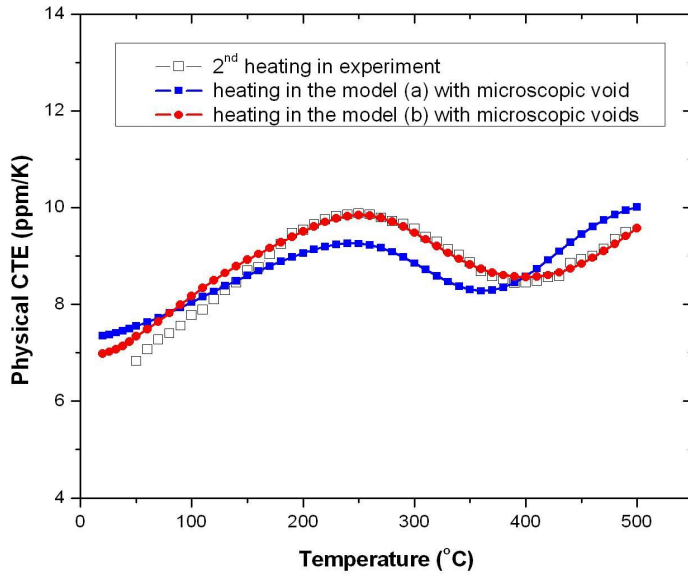

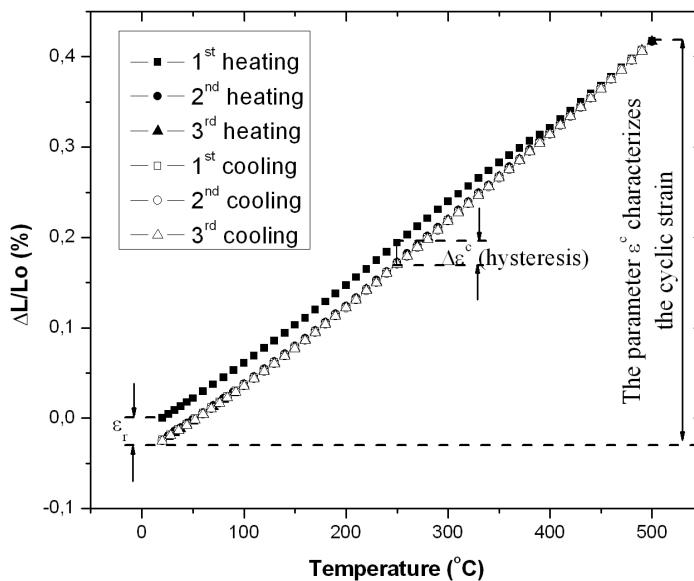Figure 6. The comparison of modelled and experimental physical CTEs curves during heating

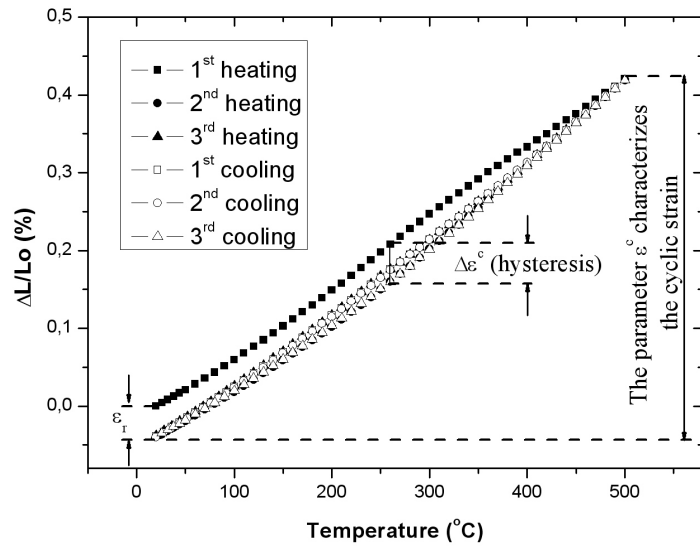Figure 7. The relative thermal expansion versus temperature of Al99.5/SiC/70p using model (a) with void

Figure 8. The relative thermal expansion versus temperature of Al99.5/SiC/70p using model (b) with voids
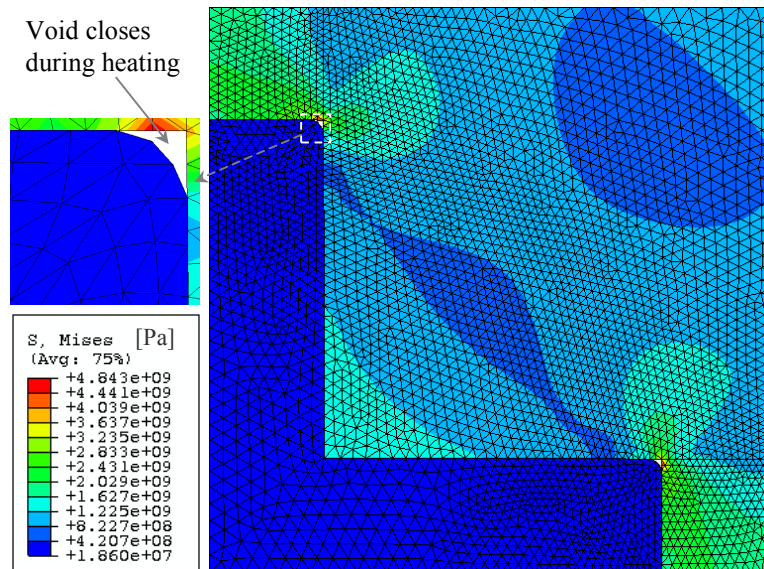

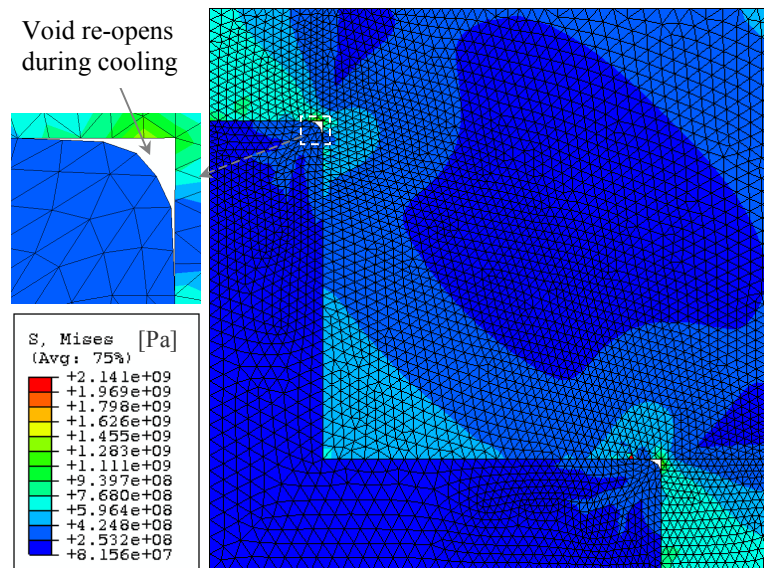Figure 9. Von Mises stress at 500°C during heating using model (b)

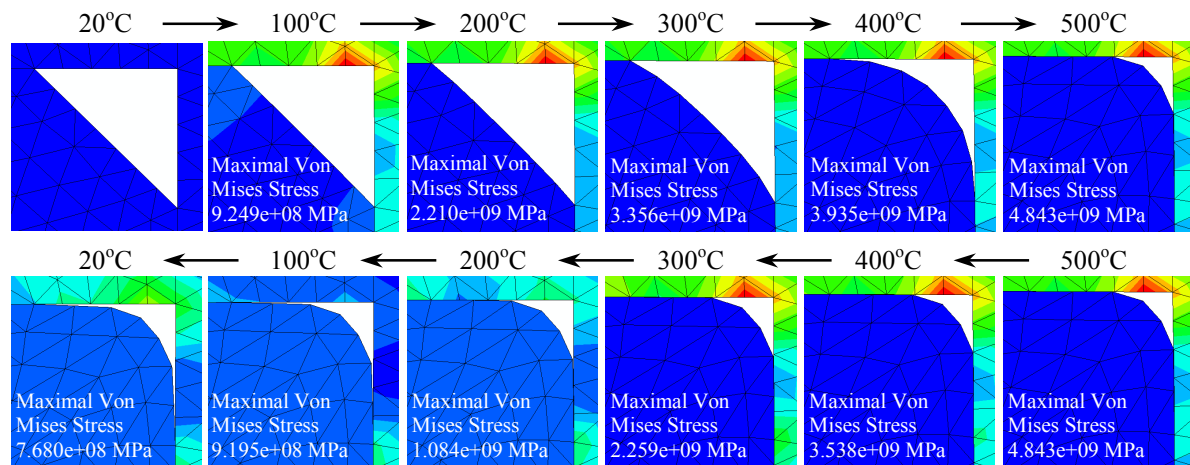Figure 10. Von Mises stress at 20°C during cooling using model (b)

Figure 11. Void closure and re-opening during heating and cooling of the investigated material using model

6   Conclusions

The coefficient of thermal expansion of an Al metal matrix with densely packed SiC particles was studied by means of numerical unit cell models between 20°C and 500°C. The unit cell models with SiC contiguity and SiC network with and without microscopic voids of an AMC reinforced with 70 vol. % SiC particles showed that the thermal expansion is strongly influenced by the presence of voids and the connectivity between the particles in the composite. The numerical results using the unit cell model (b) with voids show a good agreement with the experimental results during heating. The closure of voids by plastic flow of the matrix reduces the CTE at temperatures between 250°C and 400°C. For T > 400°C, the CTE of the composite increases again indicating that the void is filled producing again elastic straining of the constituents and confirms the hypothesis proposed by Huber et al. (2006). Experimental evidence of voids closing and opening during heating and cooling was given by synchrotron tomography of this type of AMC (Schöbel et al., 2007): the void volume fraction of 2% at RT reduced to 0.04 vol. % at 400°C.

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