NUMERICAL MODELING OF THERMAL EXPANSION OF AL-BASED METAL MATRIX COMPOSITES REINFORCED WITH SIC PARTICLES

Tran Huu Nam[1, 2], Guillermo Requena[1], H. Peter Degischer[1]

[1]Vienna University of Technology, Institute of Materials Science and Technology, Karlsplatz 13/E308, A-1040 Vienna, Austria
[2]Hanoi University of Technology, Department of Material and Structure Mechanics, No. 1, Dai Co Viet road, Hanoi, Vietnam

thnam@mail.tuwien.ac.at (Tran Huu Nam)

Abstract

The coefficient of thermal expansion (CTE) is one of the most important physical properties of metal matrix composites (MMCs). The expansion behavior is correlated to the microstructure, the deformation of the matrix, and the internal stress conditions. During the present study the instantaneous CTE of Al-based metal matrix composites reinforced with 70 vol. % SiC particles is analytically computed in order to explain abnormalities in the thermal expansion behavior obtained experimentally. The numerical modeling was carried out from room temperature (RT) to 500°C using finite element analysis (FEA) combining the effects of microscopic voids and phase contiguity. The FEA are based on a two-dimensional unit cell model. The used unit cell models consider the composites as a continuous rigid phase infiltrated with the ductile Al matrix. The obtained thermal expansion behavior is strongly influenced by the presence of voids and a comparison of instantaneous CTE with the experimental results shows a good agreement.

Keywords: Al-based metal matrix composites, Particle reinforced metals, Thermal expansion, CTE, Unit cell model.

Presenting Author's biography

Tran Huu Nam is a postdoctoral research assistant of Institute Materials Science and Technology at Vienna University of Technology. He received his Ph.D from Technical University of Liberec in Czech Republic. He is now a postdoctoral fellow of ÖAD. He is also a researcher-lecturer at Department of Material and Structure Mechanics of Hanoi University of Technology. His research interests encompass the micromechanics of composite materials, modeling and simulation of advanced materials. He is also interested in large strain materials, nonlinear properties of hyperelastic and viscoelastic materials. His present interest is thermoelastoplastic behavior of metal matrix composites.

 Copyright © 2007 EUROSIM / SLOSIM

1 Introduction

MMCs have emerged as a class of materials suitable for advanced structural, aerospace, automotive, electric, thermal management, and wear resistant applications. Al-based MMCs exhibit significant improvement in physical and mechanical properties, such as in strength, Young's modulus, fatigue resistance, tribiological properties, high-temperature mechanical properties and low thermal expansion compared with the unreinforced matrix [1-4].

Particle reinforced metals (PRMs) with high reinforcement volume fractions (> 50 vol. %) are used for thermal management applications such as electronic packaging, partly because of their excellent thermophysical properties, tailorable thermal expansion response and low density. In general, the thermal expansion behavior of a composite is the result of several material parameters: the type of constituents and the microstructure of the matrix architecture, the reinforcement volume fraction, their arrangement within the matrix, 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 [5-6].

MMCs produced by liquid-state processing where the ceramic phase is infiltrated with molten metal usually exhibit a certain degree of porosity after solidification [7]. 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 [8-9] has shown using finite element modeling that the thermal expansion is strongly influenced by the presence of voids in composites with a continuous ceramic phase. For composites with high reinforcement volume fractions, the definition of continuity of the metallic matrix becomes difficult. The ceramic can become a continuous phase as a result of specific processing methods employed. With the continuing development of high-ceramic content composites, the effects of phase contiguity as well as of microscopic voids in the material are expected to play a significant role. The presence of microscopic voids has recently been shown to strongly affect the CTE of the composites [8].

Several experimental studies have been carried out to investigate the CTE of MMCs reinforced with isolated particles [10-13]. Many theoretical models such as Turner's, Kerner's, and Schapery's have been developed to understand the thermal expansion behavior of this kind of MMCs [11-16]. Though 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 behavior of MMCs [17-23]. The thermal expansion behaviour of MMCs has been also studied numerically based on the micromechanical approach using FEM [8-9, 24-26]. Two-dimensional (2-D) unit cell models for numerical modeling of thermal expansion behavior of MMCs with high reinforcement of volume fractions based on FEA was thoroughly studied in [8]. Recently, Karadeniz and Kumlutas [17] presented representative unit cell models to study the effective coefficient of thermal expansion of fibre reinforced composites by micromechanical modeling 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 data. Chawla et al. [24] presented FEM results using the actual microstructure of aluminum reinforced with isolated SiC particles to simulate its thermal behavior. The results indicated that orientation of SiC particles changes the internal stress in the composite yielding anisotropic thermal behavior. In general most of the models employ a "unit cell" configuration, where one particle of simple shape is embedded in a continuous metallic matrix shell [17-22, 25-26].

During the present study the unit cell models are applied to analytically determine the influence of voids and interconnectivity of particles on the instantaneous CTE behavior of Al-based PRMs with high reinforcement volume fractions. In a previous experimental study of the CTE [5-6] of Al-based PRMs with 70 vol.% of interconnected and isolated SiC particles, it was proposed that the abnormalities shown by the instantaneous CTE at T > 250°C can be explained by filling and re-opening of voids during thermal cycling.

2 Materials and experimental results

2.1 Studied materials

PRMs reinforced with 70 vol. % of SiC particles using

Tab. 1 Overview of the investigated Al/SiC_p MMCs [6]

MMC designation	Matrix	Reinforcement	Fabrication process	Manufacturer	Matrix condition
Al99.5/SiC/70_p (C1)	Al99.5	SiC_p, 70 vol. %, 3-100µm	Gas pressure infiltration	Electrovac GmbH, Klosterneuburg, Austria	As cast
AlSi7Mg/SiC/70_p (C2)	AlSi7Mg				

Al99.5 (C1) and AlSi7Mg (C2) matrices were produced by gas pressure infiltration of trimodal SiC particles performs [6]. The PRMs were investigated in as cast condition. Tab. 1 lists the designation of MMCs, the ingredients, their compositions, fabrication processes as well as matrix condition. The microstructures of C1 and C2 are presented in Fig. 1 and Fig. 2. A scanning electron micrograph (SEM) of composite C2 is shown in Fig. 3, where the α-Al-phase has been removed by deep etching. "Si-bridges" between the SiC particles forming an interconnected "SiC–Si network" can be observed [7]. Such Si bridges do not exist in composite C1.

2.2 Experimental results

The CTE measurements were carried out from 20°C to 500°C using a thermo-mechanical analysis equipment (TMA 2940 CE, Thermal Instruments, USA). The specimens were machined into rectangular bars with 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 (100 ml/min). The specimen temperature was measured using a thermocouple, positioned close to the specimen [5].

Fig. 4 and Fig. 5 show the temperature dependence of the instantaneous CTEs of composites C1 and C2, respectively [6]. At lower temperatures (up to 200°C) the CTEs for the two composites vary almost linearly with the temperature. The AlSi7Mg alloy matrix expands less than the Al99.5 matrix and leads to a MMC with a generally smaller thermal expansion. A maximum in the CTE curves of the composites could be observed in the range between 200°C to 400°C. The composites yield a similar thermal behavior up to 400°C. Beyond 400°C the composite C1 shows an increase of the instantaneous CTE, whereas the CTE of composite C2 becomes constant. Only results from the 2^{nd} thermal cycle will be used for comparison, because the first heating in the experiment starts from an unknown residual stress situation.

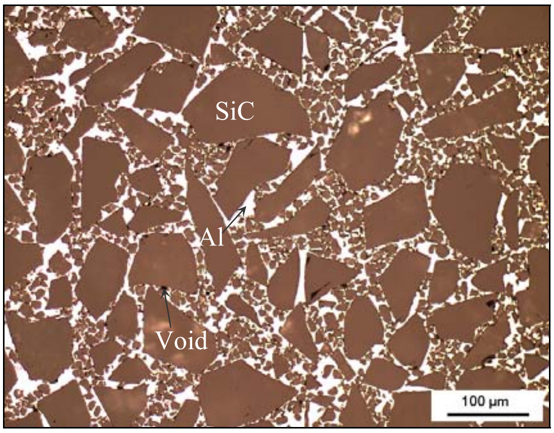

Fig. 1 Microstructure of composite C1 (Al99.5/SiC/70_p)

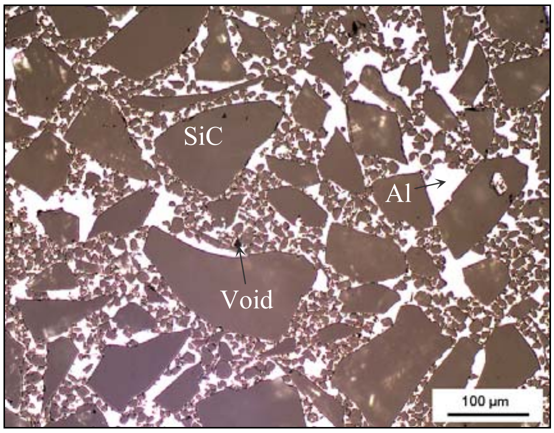

Fig. 2 Microstructure of composite C2 (AlSi7Mg/SiC/70_p)

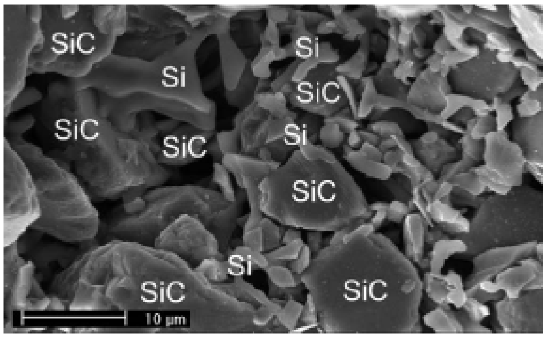

Fig. 3 The SEM micrograph of composite C2 revealing the ''Si-bridges" between the SiC particles forming a percolating "SiC–Si" network [7].

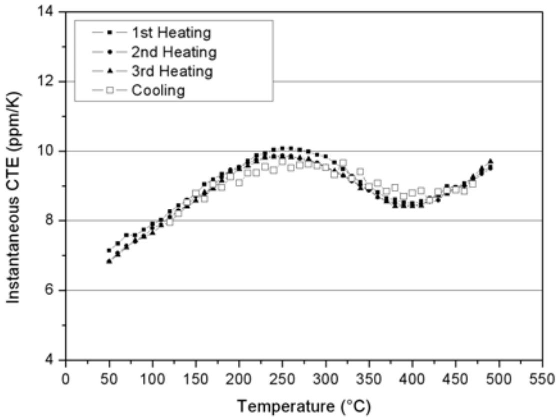

Fig. 4 The CTEs versus temperature of composite C1

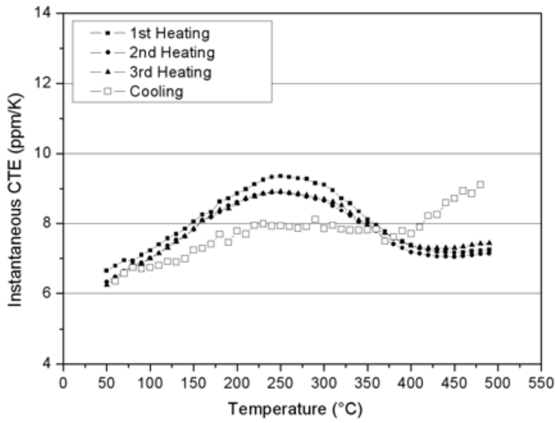

Fig. 5 The CTEs versus temperature of composite C2

ISBN 978-3-901608-32-2 Copyright © 2007 EUROSIM / SLOSIM

3 Numerical modeling

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

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

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

Two unit-cell models that feature a 2-D periodic arrangement of a discretely distributed phase of matrix embedded within the SiC contiguity and SiC-Si network as shown in Fig. 6 are proposed. Fig. 6a shows a model of SiC contiguity for modeling of composite C1. This represents the small SiC particles surrounding and contacting with the big particles in the microstructure of composite C1. The SiC-Si network of composite C2 shown in Fig. 3 is represented by the "Si-bridges" connecting the SiC particles shown in Fig. 6b. Only one quadrant of the unit cell was used for calculations due to symmetry of the geometry.

The Al alloy was considered as a strain hardening elasto-plastic solid with temperature dependent material parameters. The SiC particles and Si bridges were treated as isotropic thermo-elastic solids. The material properties for all ingredients of the investigated composites used for modeling are listed in Tab. 2. The interfaces between Al, Si and SiC were assumed to be perfectly bonded. The volume fraction of voids in modeling 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 condition). 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.

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 strain model, which normally results in a stiffer response than a full three-dimensional analysis [8]. 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. Both unit cell models are meshed using 4490 elements with 9164 nodes. The unit cells were subjected to a uniform temperature change from 20°C to 500°C.

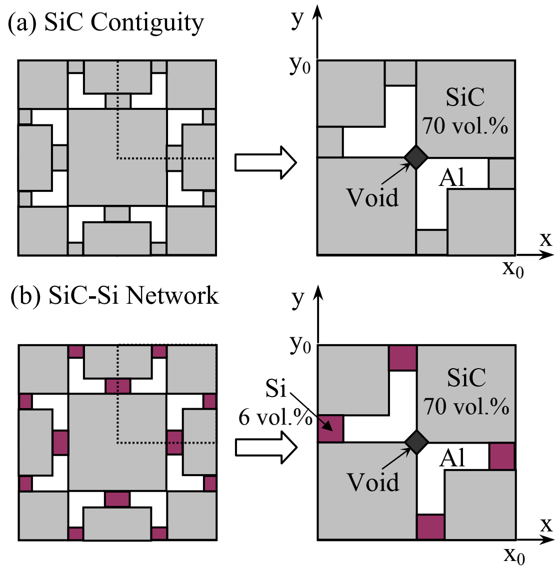

Fig. 6 Two-dimensional phase arrangements with a microscopic void: unit cell model (a) for C1 and unit cell model (b) for C2

4 Numerical results

The CTE curves during cooling and heating using

Tab. 2 The temperature-dependent elastic moduli E (GPa), Poisson ratio ν, yield stresses $\sigma_{0,2}$ (MPa) and CTE (ppm/K) of Al99.5 and AlSi7Mg matrix, SiC and Si reinforcement used for finite element modeling [6, 8, 27-28]

T (°C)	Al99.5				AlSi7Mg T5				SiC			Si		
	E	ν	CTE	$\sigma_{0,2}$	E	ν	CTE	$\sigma_{0,2}$	E	ν	CTE	E	ν	CTE
50	69.2	0.33	22.6	33.0	74.4	0.33	21.3	60.6	450	0.18	2.78	163	0.22	2.5
100	67.6	0.33	24.2	32.0	71.2	0.33	22.9	60.4	450	0.18	3.09	162	0.22	3.0
200	64.0	0.33	25.7	24.0	67.3	0.33	25.1	60.2	450	0.18	4.16	161	0.22	3.4
300	59.8	0.34	27.7	14.5	62.7	0.34	27.6	57.5	450	0.18	4.62	160	0.22	3.6
400	54.9	0.36	30.4	10.5	58.4	0.36	27.5	23.1	450	0.18	4.89	156	0.22	3.8
500	49.9	0.38	31.7	9.0	54.4	0.38	25.3	16.0	450	0.18	5.09	157	0.22	4.0

model (a) with and without void for composite C1 are shown in Fig. 7. The CTE curves during cooling and heating using model (b) with and without void for composite C2 are shown in Fig. 8. The comparison of CTE curves during heating of composite C1 and C2 is shown in Fig. 9. The experimental results of the 2nd cycle are included in Fig. 7-9 for comparison. The calculated instantaneous CTE during cooling for C1 with void (see Fig. 7) 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 modeling results are up to 1 ppm/K higher than the experimental ones. On the other hand, the calculated CTE during cooling for C2 is higher over the whole investigated temperature range (see Fig. 8).

The relative thermal expansions of composite C1 and C2 during three thermal cycles are shown in Fig. 10 and Fig. 11, respectively. 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 of thermal cycling.

The contour plots of von Mises stress at 500°C during heating for the composite C1 and C2 are shown in Fig. 12 and Fig. 14, respectively. It can be observed that the void closes during the heating of both composites. The contour plot of von Mises stress at 20°C during cooling for the composite C1 and C2 are observed in Fig. 13 and Fig. 15, respectively. 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 Fig. 16. Fig. 17 shows the maximal principal stresses of composite C1 and C2 during heating at 500°C, respectively. Compressive stresses are observed in Al matrix.

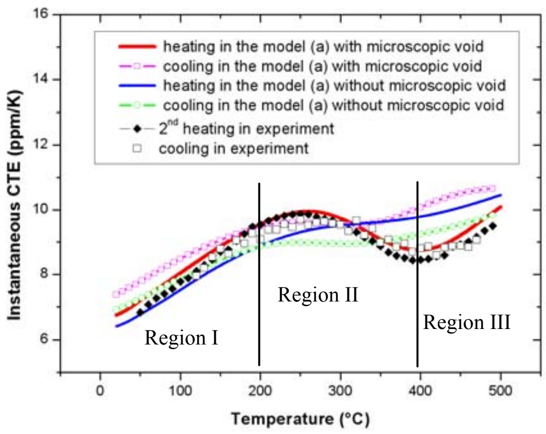

Fig. 7 The CTE versus temperature of composite C1 using model (a) with and without void compared with experimental results.

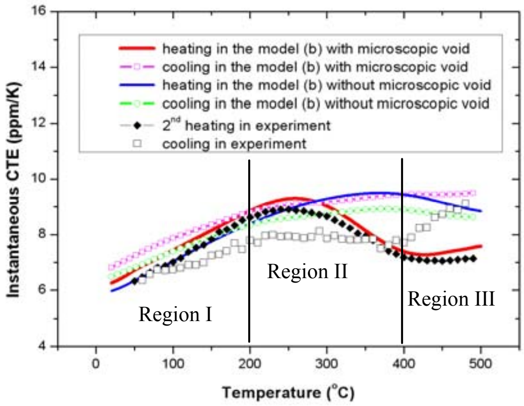

Fig. 8 The CTE versus temperature of composite C2 using model (b) with and without void.

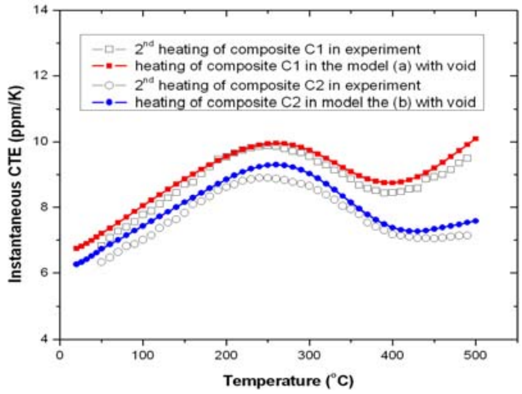

Fig. 9 The comparison of modelled and experimental CTE curves during heating of composite C1 and C2.

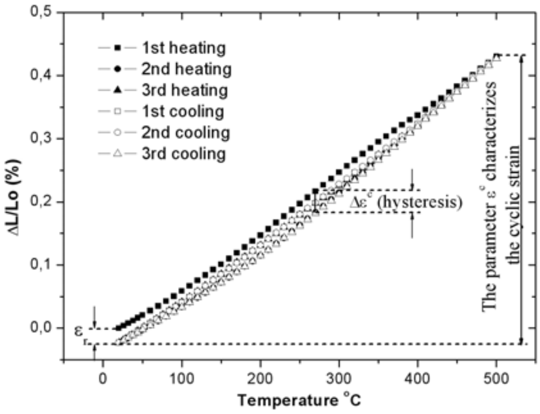

Fig. 10 Relative thermal expansion versus temperature of composite C1 using model (a) with void.

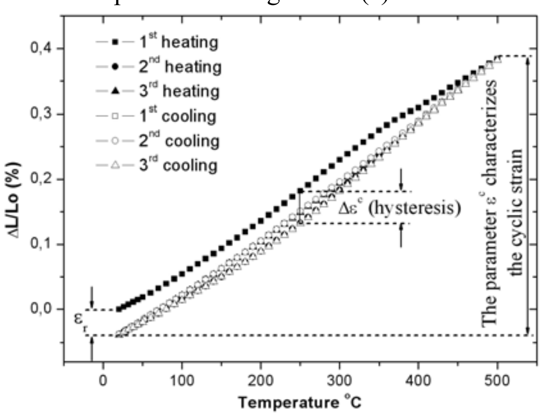

Fig. 11 Relative thermal expansion versus temperature of composite C1 using model (b) with void.

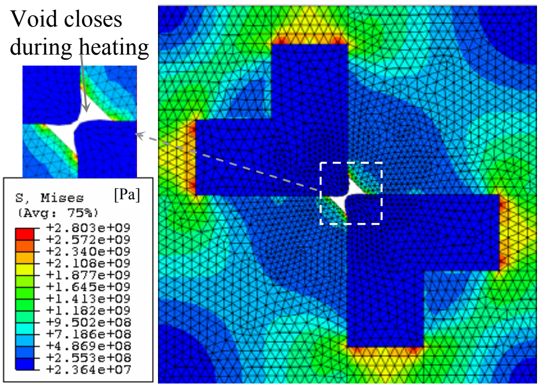

Fig. 12 Von Mises stress at 500°C during heating of composite C1.

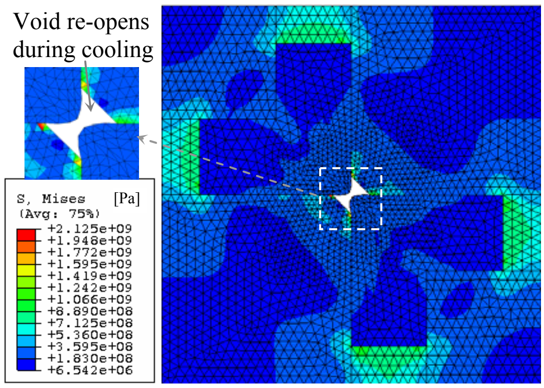

Fig. 13 Von Mises stress at 20°C during cooling of composite C1.

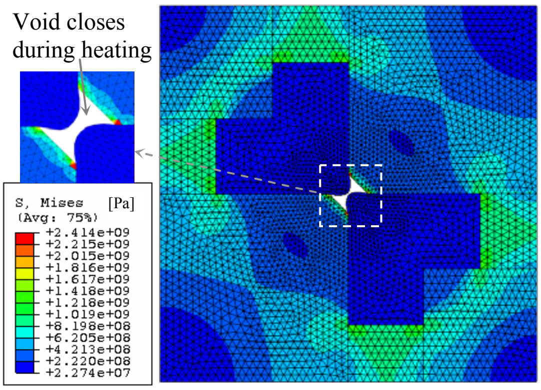

Fig. 14 Von Mises stress at 500°C during heating of composite C2.

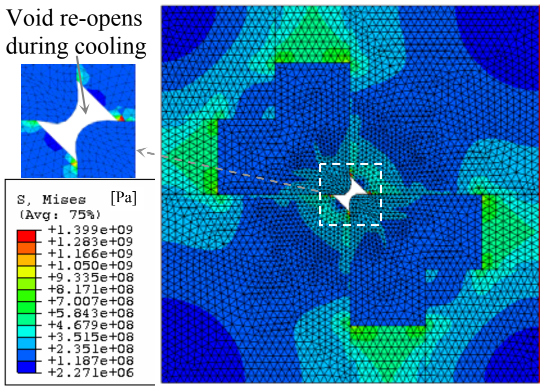

Fig. 15 Von Mises stress at 20°C during cooling of composite C2.

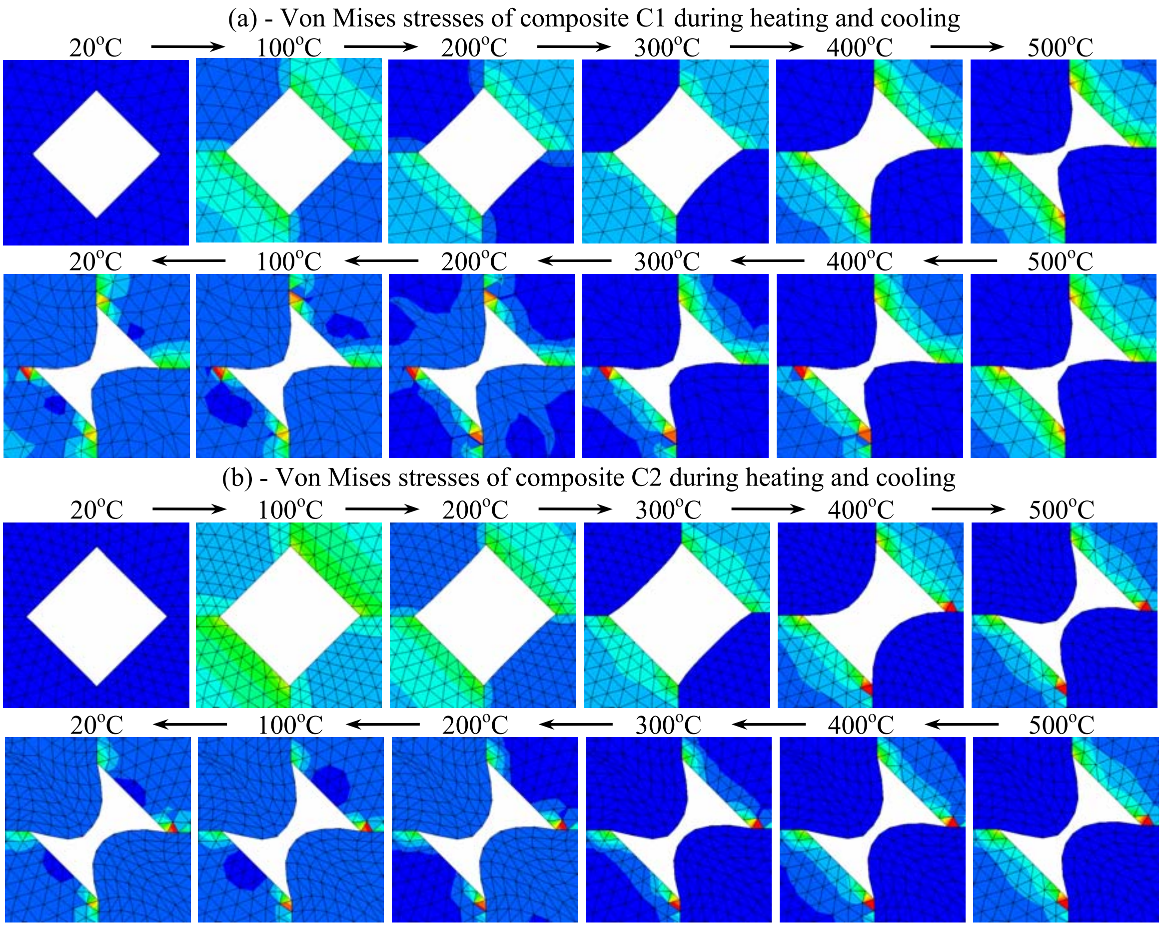

Fig. 16 Void closure and re-opening during heating and cooling of both composites

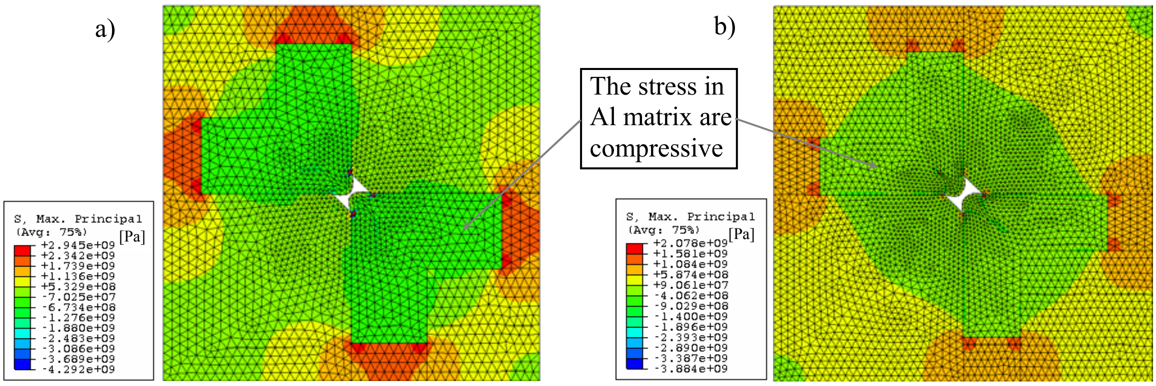

Fig. 17 Maximum principal stress at 500^{o}C during heating: (a) – composite C1, (b) – composite C2

5 Discussion of the results

The numerical results of instantaneous CTE for the model with void show a better agreement with the experiments than without void (see Fig.7-9). The CTE of both composites increases almost linearly with the temperature up to 200^{o}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. Fig. 12 to Fig. 16 showed the void closure and re-opening during heating and cooling. Von Mises stresses as observed in the Si and SiC particles as well as in the metal matrix are highest close to the SiC particles. This shows that the drop of CTE in region II of both composites is caused by the filling of voids and confirms the hypothesis proposed in [6]. In region III of Fig. 7 the composite C1 increases again indicating that the void has filled completely producing again elastic straining of the constituents [6]. The simulations show a slightly higher CTE than the experiments for temperatures > 400^{o}C. The matrix of composite C2 experiences dissolution of Si [7] within region II, which reduces the thermal expansion (Fig. 5).

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. Model (a) with void shows a good agreement with the experimental results during heating for composite C1. Model (b) is suitable for modeling of composite C2 during heating. The maximum difference of CTE between the first heating cycle of both models compared 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 presented in [14-15]. The hysteresis parameter of composite C1 and C2 using the models with void is indicated in Fig. 10 and Fig. 11. The decrease in instantaneous CTE values from 250^{o}C to 400^{o}C leads to a residual strain and hysteresis in thermal cycling curves as describes in [29].

6 Conclusions

The coefficient of thermal expansion of a SiC particles reinforced Al-based metal matrix was studied by means of numerical unit cell models between 20°C and 500°C. The unit cell models with SiC contiguity and SiC-Si network with and without microscopic voids of Al-based MMCs reinforced with 70 vol. % SiC particles showed that the thermal expansion is strongly influenced by the presence of voids. The numerical results using the unit cell model with void show a good agreement with the experimental results. The closure of voids by plastic flow of the matrix reduces the CTE at temperatures > 250°C. For T > 400°C, the CTE of the composite C1 increases again and that of the composite C2 remains nearly constant. The difference in composite C1 and C2 is essentially reduced to the different matrix alloys: the CTE of AlSi7 is smaller than that of pure aluminum and decreases above 400^{o}C due to dissolution of Si [6]. The Si bridges increase the volume fraction of the reinforcement by less than 2%. Model of C1 represents a composite with two components, whereas the geometrical similar model of C2 refers to three components.

7 Acknowledgements

The research was support by Austrian Exchange Service ÖAD (Agency for International Cooperation in Education and Research). The authors thank Prof. H.J. Böhm and Dr. Pahr for helpful discussions.

8 References

[1] F.A. Girot, J.M. Quenisset, R. Nashlain. Discontinuous-reinforced aluminum matrix composites.. *J. Comp Sci &Tech*., 30: 155-184 , 1987.

[2] J.N. Fridlymander. *Metal Matrix Composites.* Chapman and Hall Oxford, 1995.

[3] S. Elomari, M.D. Skibo, A. Sundarrajan, H. Richards, Thermal expansion behaviour of particulate metal-matrix composites, *Comp. Sci. and Technology*. 58:369-376, 1998.

[4] A. Evans, C.S. Marchi, A. Mortensen. *Metal Matrix Composites in Industry*: An Introduction and a Survey. 1st edition Springer, 2003.

[5] T. Huber. Thermal Expansion of Aluminium Alloys and Composites. *PhD Thesis*, Inst. of Materials Science and Technology, Vienna University of Technology, 2003.

[6] T. Huber, H.P. Degischer, G. Lefranc, T. Schmitt. Thermal expansion studies of aluminum-matrix composites with different reinforced architechture of SiC particles. *Comp. Sci. and Technol.*, 66:2206-2217, 2006.

[7] T. Huber, H. Knoblich, H.P. Degischer. Characte--risation of the microstructure of Al/SiCp metal-matrix composites. *Inter. J. Mater. Prep. Image Anal. Microstr.,* 40:432–42, 2003.

[8] Y.L. Shen. Combined effects of microvoids and phase contiguity on the thermal expansion of metal-ceramic composites. *Materials Science and Engineering* A237:102-108, 1997.

[9] Y.L. Shen. Thermal expansion of metal-ceramic composites: a three-dimensional analysis. *Materials Science and Engineering* A252:269-275, 1998.

[10] W.D. Frei, M. Hu, C.K. Yao. Thermal expansion and thermal mismatch stress relaxation behaviors of SiC whisker reinforced aluminum composite. *Materials Chemistry and Physics*, 77:882-888, 2002.

[11] Q. Zhang, G. Wu, L. Jiang, G. Chen. Thermal expansion and dimensional stability of Al-Si matrix composite reinforced with high content SiC. *Materials Chemistry and Physics*, 82:780-785, 2003.

[12] Q. Zhang, G. Wu, G. Chen , L. Jiang, B. Luan. The thermal expansion and mechanical properties of high reinforcement content SiCp/Al composites fabricated by squeeze casting technology. *Composites*: *Part A,* 34:1023-1027, 2003.

[13] R. Arpón, J.M. Molina, R.A. Saravanan, C. García-Cordovilla, E. Louis, J. Narciso. Thermal expansion behaviour of A/SiC composites with bimodal particle distributions. *Acta Materialia* 51:3145–3156, 2003.

[14] K.M. Shu, G.C. Tu. The microstructure and the thermal expansion characteristics of Cu/SiCp composites. *Materials Science and Engineering*, A349:236-247, 2003.

[15] S. Yu, P. Hing, A. Hu, Thermal expansion behaviour of polystyrene-aluminium nitride composites. *J. Phys. D: Appl. Phys.*, 33: 1606-1610, 2000.

[16] C.-L. Hsieh, W.-H. Tuan. Elastic and thermal expansion behavior of two-phase composites. *Materials Science and Engineering* A425: 349-360.

[17] Z. H. Karadeniz, D. Kumlutas. A numerical study on the coefficient of thermal expansion of fiber reinforced composite materials. *Composite Structures*, 78:1-10, 2007.

[18] H. Ismar, F. Schröter. Modeling and numerical simulation of the thermomechanical cyclical behavior of a cross-ply MMC. *Computational Materials Science*, 16: 259-266, 1999.

[19] M.S. Bruzzi, P.E. McHugh, F.O'Rourke, T. Linder. Micromechanical modeling of the static and cyclic loading of an Al 2124-SiC MMC. *Int. J. of Plasticity*, 17: 565-599, 2001.

[20] H.J. Böhm, A. Eckschlager, W. Han. Multi-inclusion unit cell models for metal matrix composites with randomly oriented discontinuous reinforcements. *Computational Materials Science*, 25:42–53, 2002.

[21] D.P. Mondal, N. Ramakrishnan, S. Das. FEM modeling of the interface and its effect on the elastio-plastic behavior of metal matrix composites. *Materials Science and Engineering*, A433: 286-290, 2006.

[22] P. Kenesei, A. Borbély, H. Biermann. Microstructure based three-dimensional finite element modeling of particulate reinforced metal–matrix composites. *Materials Science and Engineering*, A387: 852–856, 2004.

[23] N. Chawla, V.V. Ganesh, B. Wunsch. Three-dimensional (3D) microstructure visualization and finite element modeling of the mechanical behavior of SiC particle reinforced aluminum composites. *Scripta Materialia* 51:161–165, 2004.

[24] N. Chawla, X. Deng, D.R.M. Schnell. Thermal expansion anisotropy in extruded SiC particle reinforced 2080 aluminum alloy matrix composites. *Mater. Sci. and Eng.*, 426:314-322, 2006.

[25] R. Lázaro, H.J. Böhm. Thermal Expansion Modelling of SiC Particle reinforced Aluminium for Electronic Applications. *Internal report*, Inst. of Light Weight Structures and Aerospace Engineering, Vienna University of Technology, 2003.

[26] M. Chaturvedi, Y.L. Shen. Thermal expansion of particulate-filled plastic encapsulant: a micromechanical characterization. *Acta mater.* 46:4287-4302, 1998.

[27] J.A. King. Materials Handbook for Hybrid Microelectronics. *Artech House*, Norwood, MA, 1988.

[28] M. Bauccio. ASM Engineered Materials Reference Book, 2nd Edition. *ASM International Materials Park*, OH, 1994.

[29] S. Kumar, H. Dieringa, K.U. Kainer. Effect of particulate content on the thermal cycling behaviour of the magnesium alloy based hybrid composites. *Composites A*, 36:321-325, 2005.

ISBN 978-3-901608-32-2 *Copyright © 2007 EUROSIM / SLOSIM*