การวิเคราะห์ไฟไนต์เอลิเมนต์เชิงกลระดับจุลภาคของวัสดุเชิงประกอบที่มีโลหะเป็นเนื้อหลักซึ่งถูกเสริมความแข็งแรงด้วยอนุภาค

สุรศักดิ์ สุรนันทชัย [1]
มหาวิทยาลัยเทคโนโลยีพระจอมเกล้าธนบุรี บางมด ทุ่งครุ กรุงเทพฯ 10140

บทคัดย่อ

งานวิจัยนี้เกี่ยวข้องกับการประยุกต์ใช้การวิเคราะห์คุณสมบัติระดับจุลภาคเชิงกลด้วยไฟไนต์เอลิเมนต์ เพื่อศึกษาและสืบสวนพฤติกรรมการแปรรูปของวัสดุเชิงประกอบที่มีโลหะเป็นเนื้อหลัก โดยถูกเสริมความแข็งแรงด้วยอนุภาคเซรามิกส์ ยูนิตเซลล์ 3 มิติที่ได้รับจากรูปแบบการเกาะตัวกันของโมเลกุลเป็นลูกบาศก์อย่างง่าย ซึ่งเป็นตัวแบบจำลองในอุดมคติของวัสดุเชิงประกอบจริงประเภทนั้นที่ประกอบด้วยอนุภาคเสริมความแข็งแรงที่ถูกกระจายตัวอย่างสุ่ม (ทิศทางไม่แน่นอน) ในเนื้อโลหะหลักได้ถูกนำมาเพื่อใช้งาน สำหรับการทำให้ง่าย ดังนั้นในโครงงานวิจัยนี้อนุภาคเสริมความแข็งแรงในแบบจำลองยูนิตเซลล์ถูกสมมุติให้มีลักษณะเป็นของแข็งและมีรูปร่างทรงกลม ยูนิตเซลล์แบบลูกบาศก์ที่ถูกสร้างขึ้นได้ถูกนำมาเพื่อใช้สำหรับการทำแบบจำลองการแปรรูปของ AA6061/SiCp ที่ระดับอัตราส่วนเชิงปริมาตรของตัวเสริมความแข็งแรงต่อเนื้อโลหะหลักเท่ากับ 15 และ 20 เปอร์เซ็นต์ ภายใต้ภาระแรงดึงในแนวแกนเดียวความสัมพันธ์ของความเค้นและความเครียดที่ได้รับจากการวิเคราะห์แสดงว่า การเติมอนุภาคเสริมความแข็งแรงลงในเนื้อโลหะหลัก ช่วยปรับปรุงทั้งความแข็งเกร็งและความแข็งแรงของวัสดุเชิงประกอบให้ดีขึ้น เมื่อถูกเปรียบเทียบกับวัสดุที่ไม่ได้รับการเสริมความแข็งแรง ภาพวาดเส้นโครงร่างแสดงการแบ่งบริเวณพื้นที่ (Contour Plots) ของสนามความเค้น Mises และความเครียด Equivalent Plastic ภายในยูนิตเซลล์ ที่ได้รับจากการทำแบบจำลองในปัจจุบัน แสดงความสอดคล้องที่ดีกับผลลัพธ์ที่ได้รับโดยนักวิจัยท่านอื่นๆ

คำสำคัญ : การวิเคราะห์ไฟไนต์เอลิเมนต์เชิงกลระดับจุลภาค / แบบจำลองยูนิตเซลล์ลูกบาศก์อย่างง่าย / AA6061/SiCp / อนุภาคเสริมความแข็งแรงเป็นของแข็งและมีรูปร่างทรงกลม

---

[1] *อาจารย์ ภาควิชาวิศวกรรมเครื่องมือและวัสดุ*

Micromechanical Finite Element Analysis of Particulate-Reinforced Metal Matrix Composites

Surasak Suranuntchai [1]

King Mongkut's University of Technology Thonburi, Bangmod, Toongkru, Bangkok 10140

Abstract

This research is concerned with the application of micromechanical finite element analysis to investigate the deformation behaviour of particulate-reinforced metal matrix composites (PRMMCs). A three-dimensional unit cell from simple cubic packing as an idealisation of real composites with randomly distributed reinforcing particles in the matrix has been carried out. In the present project, the particulate in the unit cell is assumed rigid and spherical for simplicity. The cubic cell established has been employed for modelling the deformation of AA6061/SiCp at 15% and 20% volume fractions under the uniaxial tensile load. The nominal stress-strain relationship obtained from analysis has shown that the inclusion of a reinforcing phase improves both the stiffness and the strength of PRMMCs, as compared to the unreinforced material. The contour plots of the Mises stress and the equivalent plastic strain fields within the unit cell obtained from the present modelling have shown good agreements with results obtained by other researchers.

Keywords : Micromechanical FEA / Simple Cubic Unit Cell Model / AA6061/SiCp / Rigid and Spherical Particles

---

[1] *Lecturer, Department of Tool and Materials Engineering.*

1. Introduction

The finite element (FE) modelling techniques through the use of unit cell approach are customarily employed to investigate the microscopic deformation of PRMMCs, see Weissenbek et al. [1] and Banks-Sills et al. [2], for example. They attract the rapid increasing attention from materials scientists in order to achieve a better understanding of the behaviour of these composites. Owing to the fact that the distribution of particles within PRMMCs is three-dimensional in nature, idealisations of the particle arrangements in the matrix of such composites tend to give rise to a wide variety of unit cells. Consequently, the study on the packing systems of crystals has been found to be of great assistance. Many packing systems can be typically transplanted over from crystals in a straightforward manner, such as simple cubic, body-centred cubic, face-centred cubic and close-packed hexagonal packing (Nye [3]). However, only the simple cubic unit cell, which is actually known as the topologically simplest model established from Voronoi tessellation, will be used in the current exploration.

The unit cell developed for modelling the behaviour of PRMMCs will be verified by the deformation of AA6061/SiCp under uniaxial tension. The responses of the model will be validated against available published experimental data in the literature.

2. The Simple Cubic Unit Cell Model for Particulate-Reinforced Composites

In a real particulate-reinforced composite, particles are randomly dispersed in the matrix. As a result, this kind of composites might be approximated to behave isotropically in three dimensions [1]. The mechanical behaviour of the composite, in addition, is dependent on the physical properties, volume fractions and packing geometry of the constituent phase, and on the condition of the interfaces between these two phases.

For studying the structure of crystals, a range of typical idealised packing systems for composites reinforced by particles has been suggested. In these crystal packings, a large number of geometric symmetries obviously exist. It is clear that different patterns of the unit cells may be introduced by making different use of symmetries.

2.1 Voronoi Tessellation for Simple Cubic Packing System and Its Unit Cell

According to Ahuja and Schachter [4], Voronoi tessellation scheme can be employed to tessellate packing arrangements of such composites. A cell obtained from this scheme can be described as a domain enclosed by planes each of which is perpendicular to the segment connecting the centre of the grain particle and that of a neighbouring grain particle and passes through the middle point of the segment. In any a packing system, in addition, if a repetitive Voronoi cell recovers all the other cells under translational symmetry transformations, the cell can be used as the unit cell for this packing [5]. A major advantage of the development of unit cell by the application of Voronoi tessellations is that only a single particle, especially in case of simple shapes such as cylindrical, spherical and rectangular parallelepiped, will be contained in each cell.

To give an obvious visualisation, graphical illustration of the simple cubic unit cell with spherical particle has been shown in Fig. 1. A Voronoi cell for such the packing of particulate-reinforced composites appears to be a cube, in which its faces are bounded by three pairs of parallel and opposite planes in each direction of the rectangular coordinate system, i.e.

$$x = \pm b, \quad y = \pm b, \text{ and } z = \pm b \tag{1}$$

where b is defined as a half-length of each couple cell sides.

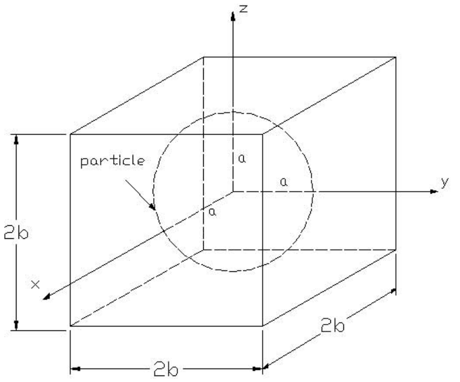

Fig. 1 A three-dimensional Voronoi unit cell for simple cubic packing of a PRMMC

Assuming particles are all of spherical shape with radius a, for a specific reinforcement volume fraction of the composite concerned, the dimension of the unit cell model in terms of b can be expressed as:

$$V_f = \frac{\pi \cdot a^3}{6 \cdot b^3}. \tag{2}$$

3. Modelling the Deformation of an Al-Alloy/SiC Particulate under Uniaxial Tension

3.1 Available Experimental Data

The composite involved in the current study is an Al-SiC PRMMC. The matrix is AA6061-T6, and the reinforcement SiC particles. Tensile stress-strain curves obtained experimentally at room temperature for three volume fractions, 0% (i.e. unreinforced), 15%, and 20%, have been presented by McDanels [6]. Also, some essential mechanical properties of the matrix alloy for computations are taken from Meijer et al. [7].

3.2 The FE Mesh and Boundary Conditions

For the FE modelling in this work, a single cube cell is taken from the bulk composite under investigation. Because of the symmetry in this cell, only one-eighth of the cubic cell is analysed, as shown in Fig. 2. The 3-D FE mesh, employed to model the unit cell, is composed of 8-noded linear brick elements with 2x2x2 Guassian quadrature in each element. With the rigid particle approximation, it is clear that the FE discretisation is required only in the matrix. When the PRMMC deforms, the localised triaxial stresses and plastic strain concentrations, several times of their nominal values, build up within the matrix, especially at the vicinity of the reinforcement-matrix interfaces [8]-[9]. Thus, the size of elements generated around these critical regions must be refined appropriately, in order that satisfactory prediction can be obtained.

With reference to Fig. 2 and based on the analysis of Agarwal and Broutman [10], the boundary conditions which must be prescribed to the current unit cell subjected to a uniaxial tension in the z-direction can be summarised as follows. By symmetry consideration of the unit cell, the macroscopic shear stresses; τ_{xy} , τ_{yz} and τ_{zx}, on all the faces of the cubic cell ABCDEFGH must be zero. Accordingly, the faces ABFE, EFGH and BCGF of the cube remain parallel to their original positions after deformation while the faces ABCD, ADHE and DCGH are constrained from normal displacement. To satisfy the perfect bonding, there must be no movement in all directions of the surface arch IJK.

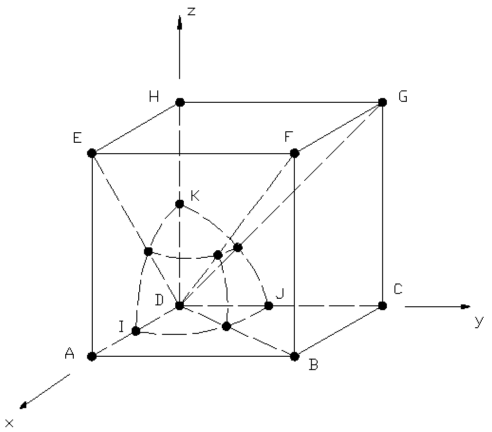

Fig. 2 The simple cubic cell employed in the present FE analyses

3.3 Computational Implementation and Solution Procedures

For analyses of these problems, a commercially available FE package ABAQUS [11] is used. In accordance with the uniaxial tension experiments conducted by McDanels [6], the tensile load applied on the top surface of the unit cell is prescribed by the boundary displacement up to a nominal strain of 5%. To obtain the elastic-plastic nominal stress-strain responses of the chosen PRMMC for two different reinforcement volume fractions: 15% and 20%, the nominal stress and strain values have to be calculated at each time-intervals. The nominal stresses are obtained by dividing the resultant force on the top boundary of the unit cell by the top surface area. In the mean time, the nominal strains can be computed directly from the prescribed displacement; i.e., the displacement of the top surface boundary divided by the original length of the unit cell.

4. Results and Discussion

The modelling results from the FE micromechanical analyses through using simple cubic unit cell to investigate the deformation behaviour of such above the PRMMC are presented and discussed in the following subsection.

4.1 The Predicted Stress-Strain Behaviour

Fig. 3 shows the predicted nominal stress-strain curves together with the experimental PRMMC material's data from McDanels [6] at reinforcement volume fractions of 15% and 20%, up to a nominal strain of 5%. Also shown in the same figure are the experimental and the predicted stress-strain curves for the unreinforced matrix material. It can be seen that the inclusion of a reinforcing phase improves both stiffness and strength of the composite, as compared to the unreinforced material. Due to rigid reinforcement assumption, the stress level for AA6061/SiCp containing 15% volume fraction of reinforcement, predicted from such the cubic cell model, tends to over predict. For strain in excess of 4%, however, the prediction is in reasonable agreement with the experimental data.

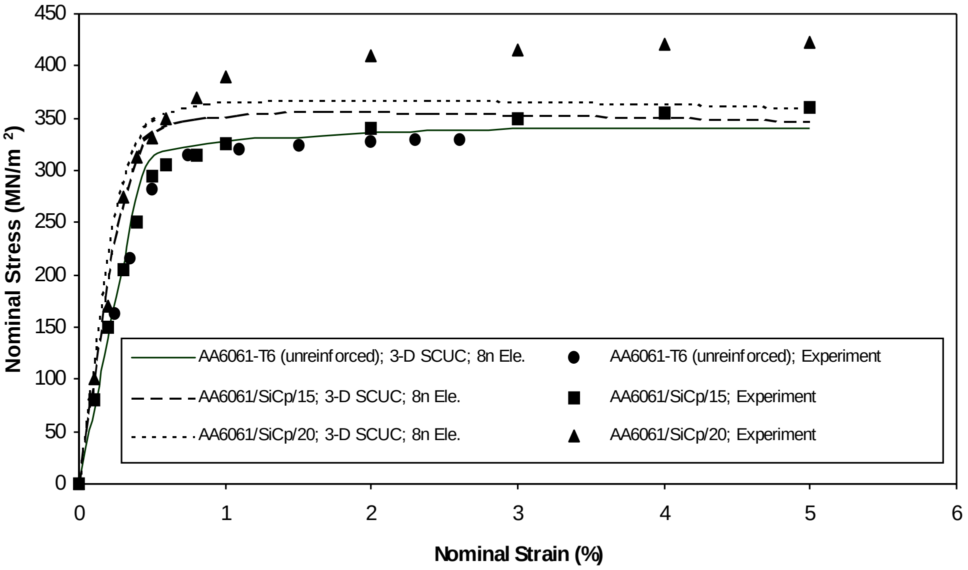

Fig. 3 Nominal stress against nominal strain curves for AA6061/SiCp containing 15% and 20% reinforcement volume fraction

It can also be seen from Fig. 3 that this assumption does not affect the prediction made for the PRMMC with 20% reinforcement volume fraction, when the strain level is greater than 0.8%. In addition, the trend of increasing discrepancy arises in this curve, as compared with the experiment, at higher levels of strain. McDanels [6] reported that for this material, damage in the form of void nucleation and growth occurred early during tensile deformation. Since material damage is not taken into account in the present FE analysis, the difference in the predicted and experimental stress-strain curves of the form shown in Fig. 3 is then expected.

4.2 Stress and Strain Fields Local to the Reinforcement

As realised that stresses and plastic strains around the reinforcement of the PRMMC are crucial for determining both the subsequent deformation behaviour and the development of damage. It is therefore important to examine the nature of the stress and plastic strain fields. Fig. 4 shows the contour plot of von Mises stress, at 5% nominal strain, for the PRMMC concerned with 15% volume fraction of reinforcement. It can be seen that a highly Mises stressed zone predicted is observed in most regions within the matrix part of the model. The high stresses bring about the increase in the overall strength and stiffness of the composite and their maximum magnitude in tension also has significant implications in terms of damage initiation and propagation in the material due to interface debonding for example [12]-[13].

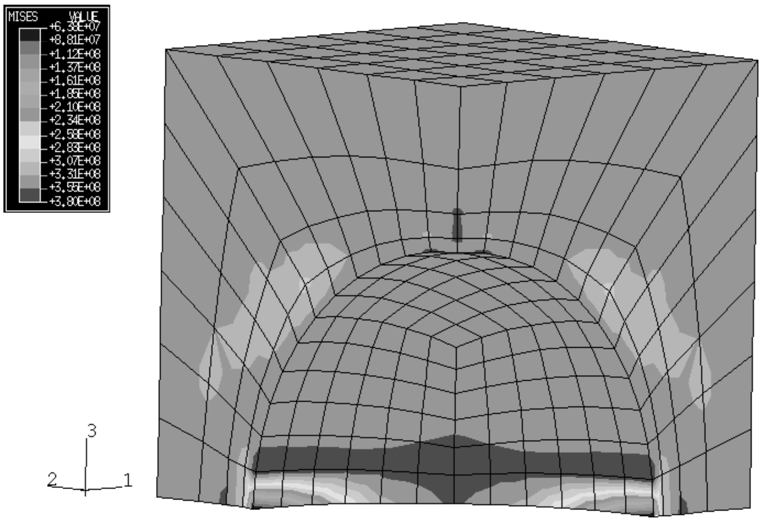

Fig. 4 Contour plot of the von Mises stress at 5% nominal strain, for AA6061/SiCp at 15% reinforcement volume fraction

Another important feature of the contour is that along the matrix-reinforcement interface, there is a gradual increase of the Mises stress level from the bottom of the cell reaching its maximum a short distance afterwards. The circumferential band of the maximum Mises stress covers a fairly wide interfacial area. In addition, high Mises stress is also found as isolated small patches in the matrix above the top of the particle close to the interface. From the Mises stress contour plot within the cubic representative cell of the composite obtained here, it is obvious that high stresses are very localised in regions around the interface and the Mises stress is approximately uniform and close to the nominal value. It is believed that the high Mises stresses local to the interface result from the constrained plastic flow. Moreover, it is interesting to note that the side-wall constraint imposed on the unit cell by the symmetry requirement may cause high tensile stresses outside the interfacial surface between matrix and reinforcement.

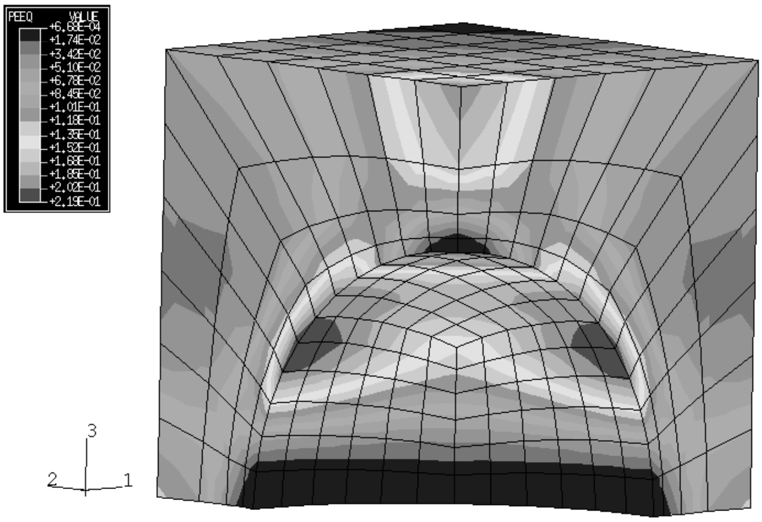

Fig. 5 Contour plot of the equivalent plastic strain at 5% nominal strain, for AA6061/SiCp at 15% reinforcement volume fraction

Fig. 5 shows the contour plot of the equivalent plastic strain for the same above material, at 5% nominal strain. From the contour plot, high equivalent plastic strain zones are observed in a region above the top of the particle around the top surface of the unit cell and also in a circumferential band halfway through the meridian around the interface. The highest level of predicted equivalent plastic strain is found on the interface at two locations, as shown in Fig. 5. The high levels of equivalent plastic strain are mainly due to the constraints introduced by the rigid reinforcement. They have significant implications in terms of damage in the PRMMC material [14].

The results obtained above are clearly related to the likelihood of damage in the form of void nucleation in the matrix or initiation and growth of interfacial debonding under the high Mises stress. The high equivalent plastic strain enhances the growth rate of existing voids. Consequently, the region in circumferential direction around the reinforcement-matrix interface is a critical site for damage initiation. This is confirmed by the uniaxial tensile tests conducted by Whitehouse et al. [14] on an Al-SiC MMC material reinforced with different types of reinforcement. They have revealed that for PRMMCs voiding occurs around the reinforcement-matrix interface and initiates near the sharp corners of reinforcements.

Comparing the present prediction of the distribution of the Mises stresses and the equivalent plastic strains with those of other researchers, such as Christman et al. [15] and Llorca et al. [8], good agreements have been obtained. This validates the predictions made in this project and the FE models adopted.

5. Conclusions

In this project, a unit cell for the simple cubic packing as an idealisation of real composites with randomly distributed reinforcing particles in the matrix has been developed under the assumption of reinforcing particles being rigid and spherical. The cubic unit cell established has been applied to modelling of the deformation of an AA6061/SiCp PRMMC at two volume fractions: 15% and 20% under the uniaxial tensile load. For simplicity, however, a number of justified assumptions for relevant factors of particles have been made in such modelling analyses. Due to the symmetries in the simple cubic cell, only one-eighth of the cell needs to be involved in the analysis, discretised by 8-noded linear brick elements with 2x2x2 points Guassian quadrature. The commercial code ABAQUS [11] has been used.

The predictions in form of the nominal stress-strain relationship have revealed that the inclusion of a reinforcing phase improves both the stiffness and the strength of PRMMCs, as compared to the unreinforced matrix material. Further, as expected, the increases in stiffness and strength depend directly on the volume fraction of reinforcement. Due to the rigid reinforcement assumption adopted, the predicted results tend to be over estimate the stiffness and strength of the PRMMC and the discrepancy gradually increases with the increase of strains, as compared with experimental data.

The contour plots of the Mises stress and the equivalent plastic strain fields within the PRMMC material during the deformation obtained from the present FE modelling using a cubic cell show good agreements with numerical and experimental results obtained by other researchers. The validity of the FE model employed is demonstrated.

6. References

1. Weissenbek, E., Bohm, H. J., and Rammerstorfer, F. G., 1994, "Micromechanical Investigations of Arrangement Effects in Particle Reinforced Metal Matrix Composites", *Computational Materials Science*, Vol. 3, No. 2, pp. 263-278.

2. Banks-Sills, L., Leiderman, V., and Fang, D., 1997, "On the Effects of Particle Shape and Orientation on Elastic Properties of Metal Matrix Composites", *Composites Part B*, Vol. 28B, pp. 465-481.

3. Nye, J. F., 1985, *Physical Properties of Crystals*, Clarendon Press, Oxford, UK.

4. Ahuja, N. and Schachter, B. J., 1983, *Pattern Models*, Wiley, New York, USA.

5. Li, S., 1999, "On the Unit Cell for Micromechanical Analysis of Fibre-Reinforced Composites", *Proc. R. Soc. Lond. A*, Vol. 455, pp. 815-838.

6. McDanels, D. L., 1985, "Analysis of Stress-Strain, Fracture, and Ductility Behaviour of Aluminum Matrix Composites Containing Discontinuous Silicon Carbide Reinforcement", *Metall. Trans. A.*, Vol. 16, No. 6, pp. 1105-1115.

7. Meijer, G., Xia, Z., and Ellyin, F., 1997, "Biaxial Cyclic Analysis of Al_2O_3p-6061 Al Composite", *Acta Mater.*, Vol. 45, No. 8, pp. 3237-3249.

8. Llorca, J., Needleman, A., and Suresh, S., 1991, "An Analysis of the Effects of Matrix Void Growth on Deformation and Ductility in Metal-Ceramic Composites", *Acta. Metall. Mater.*, Vol. 39, No. 10, pp. 2317-2335.

9. Michel, J. C. and Suquet, P., 1994, "An Analytical and Numerical Study of the Overall Behaviour of Metal-Matrix Composites", *Modelling Simul. Mater. Sci. Eng.*, Vol. 2, pp. 637-658.

10. Agarwal, B. D. and Broutman, L. J., 1974, “Three-Dimensional Finite Element Analysis of Spherical Particle Composites”, *Fibre Sci. Technol.*, Vol. 7, pp. 63-77.

11. Hibbitt, Karlsson & Sorensen, Inc., 2000, *ABAQUS/Standard Version 5.8*, USA.

12. Tvergaard, V., 1982, “On Localisation in Ductile Materials Containing Spherical Voids”, *Int. J. Fracture*, Vol. 18, pp. 237-252.

13. Tvergaard, V., 1993, “Model Studies of Fibre Breakage and Dobonding in a Metal Reinforced by Short Fibres”, *J. Mech. Phy. Solids*, Vol. 41, No. 8, pp. 1309-1326.

14. Whitehouse, A. F. and Clyne, T. W., 1993, “Cavity Formation During Tensile Straining of Particulate and Short Fibre Metal Matrix Composites”, *Acta Metall. Mater.*, Vol. 41, No. 6, pp. 1701-1711.

15. Christman, T., Needleman, A., and Susesh, S., 1989, “An Experimental and Numerical Study of Deformation in Metal-Ceramic Composites”, *Acta. Metall.*, Vol. 37, No. 11, pp. 3029-3050.