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LETTER

Three-dimensional (3D) microstructure-based modeling of crack growth in particle reinforced composites

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The mechanical properties of particle reinforced composites are largely dependent on the reinforcement particle distribution and volume fraction [1, 2]. Crack growth in particle reinforced metal matrix composites (MMCs), such as SiC particle reinforced aluminum (Al/SiC_p), is very much dependent on the reinforcement microstructure [1, 3] as well as the matrix characteristics [4, 5]. A robust numerical model to simulate crack growth must incorporate the true particle geometry, orientation, size distribution, and spatial distribution [6]. Ayyar and Chawla [6] modeled the crack growth behavior in an Al/SiC_p composite, using 2D microstructures obtained from optical microscopy. The results of these models showed that the incorporation of the "actual" microstructural attributes significantly affected the simulated crack growth response.

Of course, 2D models must be conducted under simplified stress states, such as plane stress or plane strain conditions. Thus, 2D simulations do not provide as complete a picture of the crack growth processes as 3D simulations. In reality, the stress state in 3D is quite complex. This is particularly true of composite materials, where the geometry of the SiC particle in the third dimension and the matrix around the particle play an important role. Because the geometry of the SiC particle is very complex, a 2D representation of the microstructure cannot adequately capture the behavior of the composite. Chawla et al. [7–9] have shown that predictions from 3D microstructure-based models simulating the tensile behavior of heterogeneous materials correlated well with experimental results. Most of the 3D microstructure-based modeling efforts have focused on predicting the elastic modulus and simulating the elastic-plastic behavior of the composite in tension. The onset and evolution of damage by particle fracture has been studied by a few researchers [10–14], although the reinforcement particles are modeled as simple spheres. Crack growth in 3D has not been modeled in particle reinforced metal matrix composites. In this paper, crack growth in a SiC particle reinforced Al composite was simulated, using the actual 3D microstructure of the composite.

A serial sectioning process was used to capture the complex geometry of the SiC particles from a series of micrographs of a SiC particle reinforced 2080 Al matrix composite [7, 8]. The SiC particles had a volume fraction of approximately 20%, average particle size of about 8 μm, and an average aspect ratio of 2. The serial sectioning process allows one to capture the realistic microstructure of the particles, including the geometry, orientation, and distribution of the particles. A typical flow chart of the serial sectioning and 3D reconstruction process is shown in Fig. 1. Details of this process can be found in reference [7]. The sample was cut and mounted for polishing and a "representative" region of the microstructure was selected. The term "representative" is somewhat subjective as it is dependent on the size of the SiC particles, spatial distribution, etc. As the number of particles increases, however, the computational demands also increase. For the Al/SiC_p composites modeled in this paper, a volume of about 32 particles was included in the model (which is about half of the total particles reconstructed after serial sectioning), because of reasonable limits on computational efficiency. Fiducial marks were made by Vickers indentation. These

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marks were used to measure the material thickness loss during the polishing process. The thickness removed is a function of the microstructural feature size. In this case, since the particles were approximately 6–8 μm in size, a removal rate of about 1 μm/section was selected. Using the cyclic process of polishing and imaging, it was possible to generate a series of 2D micrographs. These 2D micrographs were segmented to differentiate between the particles and the matrix. The 3D morphology of the particles was reconstructed from the series of 2D segmented images using commercially available software (SURFdriver, Kailua, Hawaii).

The 3D reconstructed microstructure was then meshed using HyperMesh® (Altair, Los Angeles, CA), Fig. 2. A 2D surface mesh was first created on the SiC particle and the Al matrix surfaces. This 2D mesh consisted of 3-node triangular elements. The 2D mesh was then used to create a 3D mesh consisting of 4-node tetrahedral elements (C3D4). The tetrahedral elements conformed well to the irregular shape of the SiC particles. A variable mesh density approach was used to reduce the overall size of the model without sacrificing the accuracy of the model. The mesh in the SiC particles and the Al matrix near the particles were finer compared to the mesh on the surfaces of the Al matrix, Fig. 2c. An embedded cell, with "average" composite properties, was used to minimize the effects of free edges. There were approximately 45,000 nodes and 240,400 tetrahedral elements (C3D4) in the model. The discretized model was then imported into a commercial finite element analysis software (ABAQUS, Pawtucket, RI). Boundary conditions were applied to the model as shown in Fig. 2d. The element elimination method was used to simulate crack growth in the particle reinforced composite. In this method an element is eliminated from the calculations when a certain parameter in the element exceeds a predefined value. The mesh was refined, since the crack profile is highly dependent on the mesh size and a fine mesh is required to obtain accurate results. Although Al is highly ductile, for the sake of simplicity, and to illustrate the feasibility of crack growth modeling using actual 3D microstructures, the Rankine criterion was used for element elimination (failure occurs when the maximum principal stress in the element is exceeded). The element elimination process, using the Rankine criterion, was simulated in the "Dynamic-Explicit" module in ABAQUS. This module requires that a mass be assigned to all the materials. Therefore, it is extremely important that the load be applied very slowly to the system to avoid any inertia effects. A velocity of 0.01 unit/s was applied to the nodes on the upper surface, as shown in Fig. 2d, until the crack had propagated through the matrix material. The value of the velocity was obtained from an iterative procedure to quantify any inertia effects. The elements in the Al matrix were eliminated when the stress reached the yield stress for the Al alloy matrix (approximately 320 MPa). Fracture of the SiC particles was not incorporated in this model, although the authors have used it in modeling 2D microstructures [15]. All three components, SiC particles, Al matrix, and the "average" composite were modeled as purely elastic. The elastic properties of SiC and Al alloy are shown in Table 1. The properties for the "Average" composite were computed using a rule-of-mixtures approach. The density was 2.81 g/cm^3, the Poisson's ratio was 0.31 and the Young's modulus was approximately 120 GPa. Particles were assumed to be bonded perfectly to the matrix. The simulation time for this model, on a DELL Precision workstation with single processor (3.0 GHz speed) and 2 GB of RAM, was approximately 6 hours.

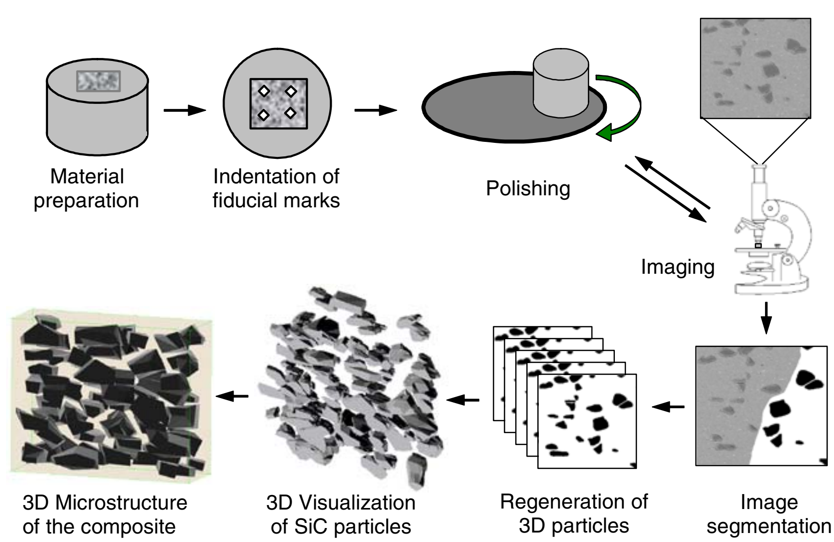

Fig. 1 A typical flow chart of the serial sectioning and 3D reconstruction process [7]

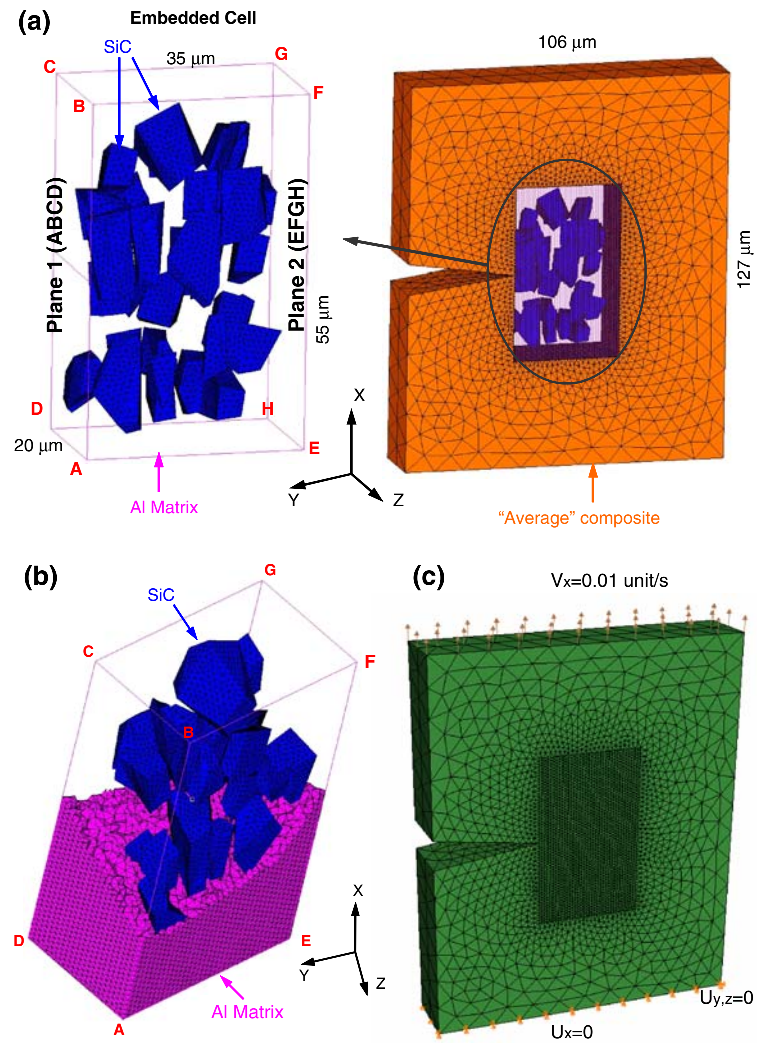

Fig. 2 (**a**) Embedded cell approach showing the 32 particle composite model. The notch provides a stress concentration point for crack initiation, (**b**) variable mesh density approach, and (**c**) boundary conditions applied to the model

Table 1 Material properties (Elastic) used in the model

Material	Density (g/cc)	Young's modulus (GPa)	Poisson's ratio
Aluminum alloy 2080-T6	2.75	74	0.33
SiC particles	3.2	410	0.19

Figure 3 shows the simulated 3D crack profile for the model of Al/SiC$_p$ composite. The model clearly shows the complex crack growth phenomenon in particle reinforced composites. The crack profile on the outer surface was very different from the crack profile on the inner surface because of the nature of the local microstructure. The crack initiates in the Al matrix along plane 1 (ABCD) and terminates in the matrix at plane 2 (EFGH). On the inner surface it was observed that the crack did not reach plane 2 (EFGH) as it was arrested by a SiC particle. Note that the crack branches around one of the SiC particles, Fig. 3b, and is forced to grow around it, Fig. 3c, as the load increases, as has been observed experimentally [1]. When particle fracture is modeled, the crack goes through the SiC particles, and the crack path is quite linear [15]. Crack growth in a homogeneous model with average composite properties, i.e., where the microstructure of the SiC particles was not explicitly considered was also modeled. The distance between plane 1 and 2, in the homogeneous model, is the same as that in the microstructure-based model. As expected, here the crack profile was planar and not very different between the outer and inner surfaces. When one incorporates the explicit microstructure, it is quite clear that the crack profile through the SiC particles is captured. The tortuous nature of crack growth, as well as the deflection of the crack due to particles can be seen. Crack deflection, of course, reduces the crack-tip driving force of the material. The applied load is plotted versus the nodal displacements for both models (microstructure-based model and homogeneous model) in Fig. 4. The crack initiates at plane 1 (ABCD) and ends at plane 2 (EFGH).

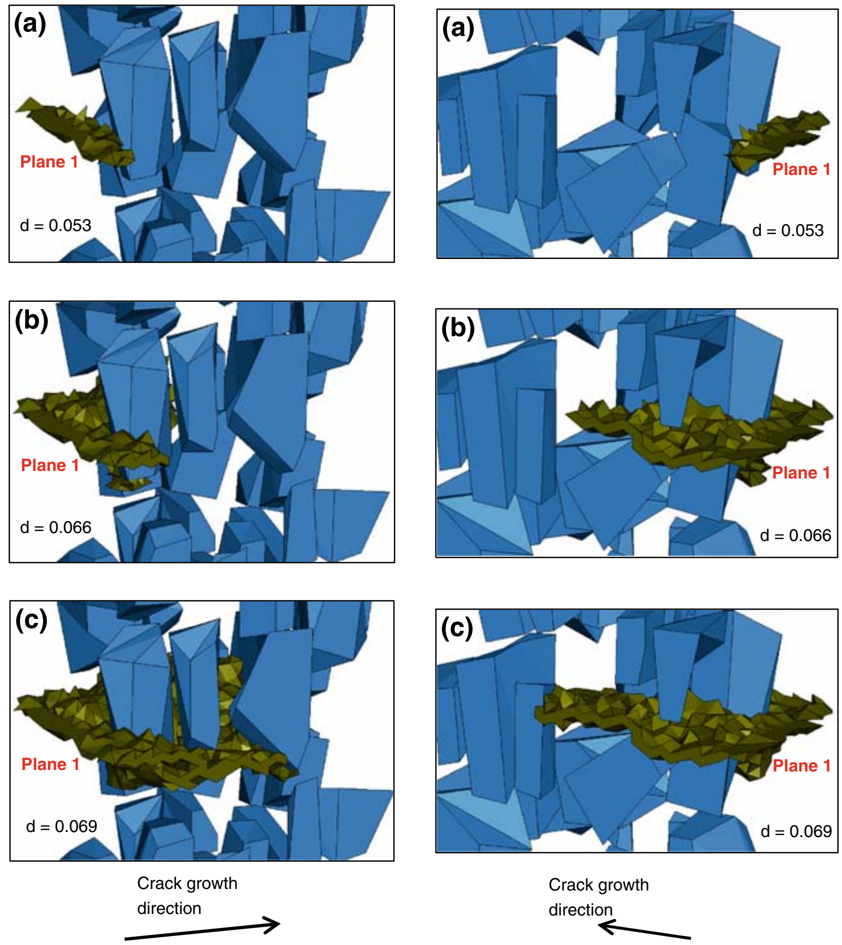

Fig. 3 3D microstructure-based simulation of crack growth showing crack arrest, crack deflection, and tortuous 3D crack surface

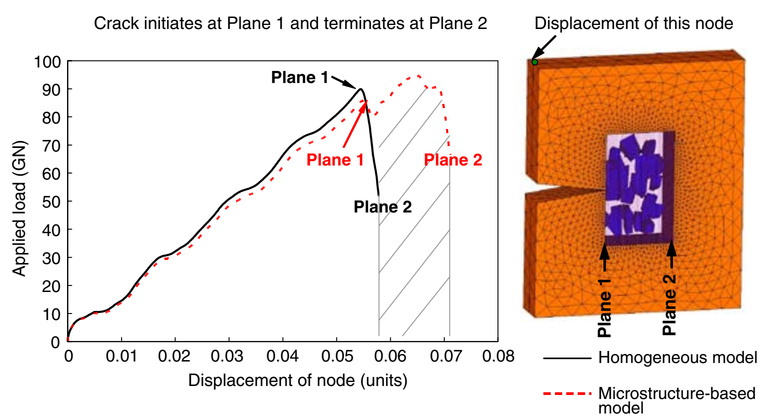

Fig. 4 Load versus displacement plots. In the microstructure-based model more energy is required to propagate the crack through the same distance (from Plane 1 to Plane 2)

Clearly, more energy was required for the crack to propagate in the microstructure-based model. This is a result of crack deflection and crack arrest by the particles in the microstructure-based model.

In summary, a 3D microstructure-based model was developed to study crack growth in Al/SiC$_p$ composites. The complex geometry of the SiC particles, in all three dimensions, was captured using a serial sectioning approach. Three-dimensional crack growth is a complex phenomenon, which involved crack deflection and crack arrest. A complex and tortuous 3D crack profile was simulated (assuming no particle fracture), which cannot be adequately represented using conventional 2D representations. This crack deflection due to reinforcement particles makes the crack path tortuous and improves the crack growth resistance of the composite.

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References

1. Chawla N, Chawla KK (2006) Metal matrix composites. Springer, New York
2. Divecha AP, Fishman SG, Karmakar SD (1981) J Metals 9:12
3. Shang JK, Yu WK, Ritchie RO (1988) Mater Sci Eng A102:181
4. Bonnen JJ, You CP, Allison JE, Jones JW (1990) In: Proceedings of the international conference on fatigue. Pergamon Press, New York, p 887
5. Sugimura Y, Suresh S (1992) Metall Trans A 23:2231
6. Ayyar A, Chawla N (2006) Compos Sci Technol 66:1980
7. Chawla N, Ganesh VV, Wunsch B (2004) Scr Mater 51:161
8. Chawla N, Sidhu RS, Ganesh VV (2006) Acta Mater 54:1541
9. Chawla N, Sidhu RS (2007) J Mater Sci-Mater Electron 18:175
10. Han W, Eckschlager A, Bohm HJ (2001) Compos Sci Technol 61:1581
11. Bohm HJ, Eckschlager A, Han W (2002) Comput Mater Sci 25:42
12. Eckschlager A, Han W, Bohm HJ (2002) Comput Mater sci 25:85–91
13. Segurado J, Gonzalez C, Llorca J (2003) Acta Mater 51:2355
14. Segurado J, Llorca J (2006) Mech Mater 38:873
15. Ayyar A, Chawla N (2007) Acta Mater (in press)