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3D micromechanical analysis of thermo-mechanical behavior of Al_2O_3/Al metal matrix composites

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ABSTRACT

In this paper an elastoplastic finite element model for studying the thermomechanical behavior of Al/Al_2O_3 particulate composites is proposed. 3D representative volume elements (RVEs) are created to model the microstructures of Al/Al_2O_3 composites and the finite element models generated from RVEs are used to study the mechanical and thermal expansion properties. In order to study the effect of thermal residual stresses, first the RVEs are simulated for cooling process from sintering temperature to room temperature and thermal residual stress are estimated for different mechanical behaviors of Al matrix. Next, the thermomechanical properties are examined with existing residual stresses. The predicted effective elastic moduli and the coefficient of thermal expansion are compared with the experimental results reported in literature. The FE results have good correlation with the experimental data and the effects of microstructural parameters, voids and properties of the constituents are further discussed. In order to study the influence of voids on the elasto-plastic behavior of composites, the Gurson–Tvergaard–Needleman (GTN) model is applied. The nucleation and growth of voids in composites, under uniaxial tension, is studied.

1. Introduction

Aluminum–alumina particle reinforced composites have been studied in detail [1–5], because of their increasing usage in high temperature structural applications requiring increased wear resistance. Simulating the thermomechanical behavior of these composites is relevant to a wide variety of applications. The thermomechanical behavior of composites is influenced by the microstructural morphologies, distribution of the constituents, and the processing methods. Modeling the behavior of high performance materials requires a thorough understanding and careful analysis of the microstructure of these materials. This can be further challenging due to the inhomogeneous and multiphase composition of the most high performance composites. Different micromechanical models have been reported to simulate the deformation behavior of metal matrix composites.

In order to incorporate the detailed information about microstructural morphologies, scanning electron microscopic (SEM) images are used for finite element mesh generation in one type of analysis [6–13]. Sharma et al. has predicted the effective Young's modulus and linear thermal expansion coefficient (CTE) of particle reinforced and interpenetrating phase composites using object oriented finite element method (OOF) [6,7]. OOF has the advantage of incorporating the real microstructure of composites, but, it conducts only 2D linear analysis [10]. The second class of micromechanics models considers simpler microstructural geometries such as spherical or ellipsoidal shaped particles distributed in the homogenous matrix [14–19] and a 3D finite element analysis is conducted. A representative volume element (RVE) is obtained for such analysis from the homogenized sample of material. The goal of the homogenization approach is to provide data which can be used to find a material model for the effective material, and to identify the parameters introduced in this material model. The effective material is supposed to represent all macroscopic properties of the micro heterogeneous material. An effort is also made to simulate the realistic 3D microstructure from SEM images of composites [13,20]. Zhang et al. has reported the 3D FEM analysis of particle reinforced SiC/Al metal matrix composites (MMCs) by employing realistic microstructure (RM). 3D structures of SiC are obtained by extruding the 2D geometrical shape of SiC particle based on SEM images and these particle are randomly distributed in RVEs model material microstructure.

Apart from material microstructure, the thermo-mechanical behavior of MMCs is also influenced by some other parameters such the mismatch of CTE of constituents of composite and the

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plastic deformation of metal matrix. Residual stresses develop in metal matrix composites during the cooling process from the sintering temperature to room temperature due to CTE mismatch of constituents. Gudlur et al. have reported [21] the 2D analysis of particle reinforced metal matrix composites considering the effect of residual stresses and concluded that the elastic and thermal properties of Al/Al_2O_3 composites depend not only on the compositions and properties of the constituents, but also on the processing conditions that could lead to existence of thermal residual stresses and localized stresses due do discontinuities in geometries and constituents. Thermal residual stresses generated during fabrication process can sometimes even higher than the mechanical stresses because of the applied load [22,23]. Neutron diffraction methods are used by researchers [22,23] to determine the residual stresses that develop during the fabrication process of the Al–SiC composite. It is being reported that the matrix is in net tension and the reinforcement is in net compression because of these residual stresses. The tensile test conducted on this sample reveals that the plastic deformation actually releases these stresses [23]. Metal matrix composites fabricated using powder processing techniques often contain porosities that can influence the effective material properties. Gurson proposed [24,25] a model of void growth in a rigid-perfectly plastic matrix and this model was modified by Tvergaard and Needleman [26,27] to completely model void growth, nucleation and coalescence in ductile deformation of porous materials.

In this manuscript, the effects of microstructural morphologies, i.e., the size, shape, distribution, and properties of the constituents, existences of voids, and the presence of thermal residual stresses are studied, on the effective Young's modulus and effective CTE of $Al–Al_2O_3$ composites. The Gurson–Tvergaard–Needleman (GTN) model is used to study the elastoplastic behavior and nucleation and growth of voids of the MMCs considering micro-voids located in the aluminum phase. The three-dimensional finite element simulations are conducted for this purpose by generating the RVEs of composites. Initially the effect of microstructural parameters, i.e. the RVE's size and the mesh sensitivity analysis is conducted. The generated RVEs are exported to the commercial software Abaqus for meshing and subsequent analysis. The results obtained are compared with the experimental results reported by Gudlur et al. [28].

2. Gurson–Tvergaard–Needleman model

For a metal having dilute concentration of voids, Gurson [24,25] proposed a yield condition subjected to void volume fraction. This was later modified by Tvergaard [26] and was defined as:

$$\Phi = \left(\frac{q}{\sigma_y}\right)^2 + 2q_1 f \cosh\left(-q_2\frac{3p}{2\sigma_y}\right) - (1 + q_3 f^2) = 0 \tag{1}$$

where $q = \sqrt{\frac{3}{2}\mathbf{S}:\mathbf{S}}$ is the von Mises stress and

$$\mathbf{S} = p\mathbf{I} + \sigma,\ p = -\frac{1}{3}\boldsymbol{\sigma}:\mathbf{I} \tag{2}$$

S is the deviatoric part of the Cauchy stress tensor and p is the hydrostatic pressure σ_y is the yield stress of void free matrix material and q_1, q_2 and q_3 are the material parameters.

Pressure in the yield condition generates non-deviatoric plastic strains. Plastic flow is assumed to be normal to the yield surface:

$$\dot{\varepsilon}^{pl} = \dot{\lambda}\frac{\partial \Phi}{\partial \boldsymbol{\sigma}} \tag{3}$$

where $\dot{\lambda}$ is the plastic consistency parameter. The equivalent plastic strain's evolution in the matrix material is obtained from the following equivalent rate of plastic work expression:

$$(1-f)\sigma_y\dot{\bar{\varepsilon}}^{pl}_m = \boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}^{pl} \tag{4}$$

The total change in volume fraction of voids is defined as:

$$\dot{f} = \dot{f}_g + \dot{f}_n \tag{5}$$

where $\dot{f}_g$ is the change due to growth of existing voids and $\dot{f}_n$ is the change due to nucleation of new voids. Tvergaard suggested [26] that the nucleation of the new voids occurs mainly at the second-phase particles, by decohesion of the particle–matrix interface or by particle fracture and if it is only controlled by the plastic strain, the relation between them can be described by

$$\dot{f}_n = A\dot{\bar{\varepsilon}}^{pl}_m \tag{6}$$

where A gives the dependence of the void nucleation rate on the matrix effective plastic strain increment [27]

$$A = \frac{f_N}{S_N\sqrt{2\pi}}\exp\left[-\frac{1}{2}\left(\frac{\bar{\varepsilon}^{pl}_m - \varepsilon_N}{S_N}\right)^2\right] \tag{7}$$

where ε_N and S_N represents the mean value and standard deviation for the normal distribution of the nucleation strain, and f_N is the volume fraction of the nucleating voids [27].

3. Three- dimensional (3D) FEM analysis

We have analyzed the effective Elastic Modulus and CTE of particle reinforced composites, having 5 vol% and 10 vol% alumina reinforced in Al matrix. Gudlur et al. have reported the fabrication and analysis of Al/Al_2O_3 composites [28]. The composite specimens were produced using powder processing techniques. The alumina and aluminum powders are mixed, ball milled and cold pressed using a cold press for 30 min at room temperature. The cold pressed pallets were further sintered at 600 °C in a quartz furnace for 2 h and cooled back to room temperature. The detailed procedure can be seen elsewhere [28].

3.1. Microstructure simulation

Three dimensional RVEs of composites were generated, to represent the microstructure of 5 vol% and 10 vol% composites using Digimat software that uses a random sequential adsorption algorithm [25] for particle distribution. In modeling the MMC's microstructure, simplified geometries have been used [26–28]. However, it can be understood that such simplified geometries such as ellipsoid or spherical shape particles do not accurately represent the shape of inclusions. Also, it is reported [29] that the particulate composites with spherical shape particles tends to show higher strength than the ones with irregular shape particles. Therefore, this study is carried out using icosahedron shaped particles for the reinforcement phase. Icosahedron is a polyhedron having 20 faces and is used to model the irregular shaped alumina particles.

Initially, four different RVE's size with edge lengths: 0.25, 0.50, 0.75 and 1 mm were used to study the relative variation of thermo-mechanical properties, which is discussed ahead in this manuscript. The XRD analysis of 5 vol%, and 10 vol% alumina composite samples was reported to have the 9.4 vol% and 13.9 vol% alumina in samples [24]. This is due to the fact that the aluminum powder already contained 2.4–3.4 vol% of alumina and also some aluminum would have been oxidized during the manufacturing process [28]. Therefore, in the baseline model, the volume fraction of reinforcement is selected as 9.4 vol% and 13.9 vol % for the 5 vol% and 10 vol% alumina composites, respectively. Thirty particles with aspect ratio of 1 were used for reinforcement phase (see Fig. 1). Linear elastic and elasto-plastic material behavior with temperature dependent and temperature independent