Clustering in Zirconium Oxide/AA1100 Alloy Particle-Reinforced Metal Matrix Composites

1 S. Madhav Reddy and A. Chennakesava Reddy²

¹Research Scholar, Department of mechanical Engineering, Osmania University, Hyderabad, India. ²Associate Professor, Department of Mechanical Engineering, Vasavi College of Engineering, Hyderabad, India dr_acreddy@yahoo.com

Abstract: *In the present work, the zirconium oxideAA3003 metal matrix composites were fabricated at 10%, 20% and 30% volume fractions of zirconium oxide. The micromechanical modeling of composites was carried out with and without clustering of zirconium oxide particles in AA1100 alloy matrix. The microstructure of zirconium oxide/AA3003 alloy reveals the occurrence of particle clustering. The normalized tensile strength and elastic modulus decrease with clustering of zirconium oxide particles.*

Keywords: *AA1100, Zirconium oxide, spherical nanoparticle, RVE model, finite element analysis, clustering.*

1. INTRODUCTION

Particulate reinforced metal matrix composites are cost-effective alternatives and have the advantage of being machinable and workable using conventional processing methods. Random but non-homogeneous particle distributions arise during composite processing for several reasons. In cast metal-matrix composites, particle clustering (figure 1) is due to the combined effect of reinforcement settling and the rejection of the reinforcement particles by the matrix dendrites while these are growing into the remaining liquid during solidification [1]. Although there is a qualitative understanding of the effects of clustering on the mechanical properties of composites, a quantitative assessment cannot be made in the absence of a detailed micromechanical modeling. One of the objects of micromechanics is the prediction of macroscopic modulus of heterogeneous materials when the elastic properties of their individual phases are given [2]. In most cases such investigations are carried out by the application of Finite Element Method (FEM) [3]. In FEM numerical models very fine meshes need to be applied inside and around the inter-phase layers which results in large number of degrees of freedom. In these models the concept of repeating unit cell with a regular distribution of inclusions is usually employed [4-9].

Figure 1: Distribution of particles: (a) without clustering and (b) with clustering.

The objective of this paper is to study the effect of particle clustering on interface debonding and particle fracture using the finite element method (FEM). The shape of zirconium oxide nanoparticle considered in this work is spherical. The periodic particle distribution was a square array. Two models were used in the computational framework. The first one is uniform distribution of nanoparticles without clustering. The second one is uniform distribution of nanoparticles with clustering.

2. MATERIALS METHODS

The matrix material was AA1100 alloy. The reinforcement material was zirconium oxide $(ZrO₂)$ nanoparticles of average size 100nm. $ZrO_2/AA1100$ alloy composites were fabricated by the stir casting process and low pressure casting technique with

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argon gas at 3.0 bar. The composite samples were give solution treatment and cold rolled to the predefined size of tensile specimens. The heat-treated samples were machined to get flat-rectangular specimens (figure 2) for the tensile tests. The tensile specimens were placed in the grips of a Universal Test Machine (UTM) at a specified grip separation and pulled until failure. The test speed was 2 mm/min. A strain gauge was used to determine elongation. In the current work, a unit cell comprising of nine particles was implemented to analyze the tensile behavior zirconium oxide/AA1100 composites at three (10%, 20% and 30%) volume fractions of $ZrO₂$ and at different temperatures. The large strain PLANE183 element was used in the matrix in all the models. In order to model the adhesion between the matrix and the particle, a CONTACT 172 element was used. The discretization a unit cell without clustering of $ZrO₂$ particles is shown in figure 2a and that with clustering of $ZrO₂$ particles is shown in figure 2b.

Figure 2: The interphase in a nanoparticle-reinforced composite: (a) without clustering and (b) with clustering.

Figure 3: Tensile testing: UTM with temperature controlled chamber and (b) shape and dimensions of tensile specimen.

Considering adhesion, formation of precipitates, particle size, agglomeration, voids/porosity, obstacles to the dislocation, and the interfacial reaction of the particle/matrix, the formula for the strength of composite [10, 11] is stated below:

$$
\sigma_{\rm c} = \left[\sigma_{\rm m} \left\{ \frac{1 - \left(v_{\rm p} + v_{\rm v} \right)^{2/3}}{1 - 1.5 \left(v_{\rm p} + v_{\rm v} \right)} \right\} \right] e^{\rm m_{p} \left(v_{\rm p} + v_{\rm v} \right)} + \text{kd}_{\rm p}^{-1/2} \tag{1}
$$
\n
$$
k = E_m m_m / E_p m_p
$$

where, v_v and v_p are the volume fractions of voids/porosity and nanoparticles in the composite respectively, m_p and m_m are the possion's ratios of the nanoparticles and matrix respectively, d_p is the mean nanoparticle size (diameter) and E_p and E_p is elastic moduli of the matrix and the particle respectively. Elastic modulus (Young's modulus) is a measure of the stiffness of a

material and is a quantity used to characterize materials. Elastic modulus is the same in all orientations for isotropic materials. Anisotropy can be seen in many composites.

The upper-bound equation is given by

$$
\frac{E_c}{E_m} = \left(\frac{1 - v_v^{2/3}}{1 - v_v^{2/3} + v_v}\right) + \frac{1 + (\delta - 1)v_p^{2/3}}{1 + (\delta - 1)(v_p^{2/3} - v_p)}\tag{2}
$$

The lower-bound equation is given by

$$
\frac{E_{\rm c}}{E_{\rm m}} = 1 + \frac{v_{\rm p} - v_{\rm p}}{\delta / (\delta - 1) - (v_{\rm p} + v_{\rm v})^{1/3}}
$$
(3)

where, $\frac{\partial E}{\partial p}$ $\frac{E}{m}$

The transverse modulus is given by

$$
E_{t} = \frac{E_{m}E_{p}}{E_{m} + E_{p}(1 - v_{p}^{2/3})/v_{p}^{2/3}} + E_{m}(1 - v_{p}^{2/3} - v_{v}^{2/3})
$$
\n(4)

3. RESULTS AND DISCUSSION

The optical micrograph as shown in figure 3 reveals random distribution of $ZrO₂$ (20% Vp) particles in AA1100 alloy matrix. The clustering of particles is also seen in the microstructure.

Figure 4: Microstructure showing distribution of 20% ZrO₂ nanoparticles in AA1100 alloy matrix.

Figure 5: Effect of volume fraction on (a) normalized strength, (b) normalized tensile elastic modulus and (c) normalized shear modulus of $ZrO₂/AA1100$ composites.

Figure 5a represents the tensile stresses induced in the composites along the load direction. The tensile stresses induced in the composites were normalized with tensile strength of AA1100 alloy matrix. The results obtained from the finite element analysis (FEA) are higher than those obtained from the mathematical expression mentioned in Eq.(1) and the experimental procedure. For the case without clustering of ZrO₂ particles, the tensile stress increases with increase of volume fraction of $ZrO₂$ in AA1100 alloy matrix. But, the tensile stress decreases with increase of volume fraction of $ZrO₂$ in AA1100 alloy matrix in the case of clustering of ZrO₂ particles. The normalized elastic modulus increases with increase of volume fraction of non-clustered $ZrO₂$ particles in AA1100 alloy matrix; while it decreases with increase of volume fraction of clustered $ZrO₂$ particles in AA1100 alloy matrix (figure 5b). The normalized stiffness values obtained from FEA are within the upper bound and lower bound values computed from Equations (2) and (3), respectively. The normalized shear modulus is unaffected by the clustering of $ZrO₂$ particles as seen from figure 5c.

Figure 6: Criterion for interfacial debonding (a) and for particle fracture (b).

Figure 7: Images of von Mises stresses obtained from FEA: (a) without clustering and (b) with clustering.

If the particle deforms in an elastic manner (according to Hooke's law) then,

$$
\tau = \frac{n}{2}\sigma_p \tag{5}
$$

where, *n* is a dimensionless constant given by:

$$
n = \left[\frac{2E_m}{E_p(1+v_m)ln(1+v_p)}\right]^{1/2}
$$

 σ_p is the particle stress.

For the interfacial debonding/yielding to occur, the interfacial shear stress reaches its shear strength:

$$
\tau=\tau_{max}
$$

 $\tau = \tau_{\text{max}}$ (6) For particle/matrix interfacial debonding [12-19] can occur if the following condition is satisfied:

$$
\tau_{\text{max}} < \frac{\text{no}_p}{2}
$$

It is observed from figure 6a that the interfacial debonding occurs between ZrO_2 nanoparticle and AA1100 alloy matrix as the condition in Eq.(7) is satisfied.

 (7)

If particle fracture occurs when the stress in the particle reaches its ultimate tensile strength, $\sigma_{p,uts}$, then setting the boundary condition at

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 $\sigma_p = \sigma_{p,\;uts}$ (8) The relationship between the strength of the particle and the interfacial shear stress [12-19] is such that if $\sigma_{\rm P,uts} < \frac{2\tau}{n}$

(9)

 $\mathbf n$ Then the particle will fracture. From the figure 6b, it is observed that the $ZrO₂$ nanoparticle was not fractured as the condition in Eq. (9) is not satisfied. As seen from figure 8 the von Mises stress induced at the interface are higher than that induced in the nanoparticle. Hence, the interfacial debonding was occurred between the particle and the matrix. The interfacial debonding decreases with increase of volume fraction of ZrO₂.

4. CONCLUSION

The microstructure of $ZrO_2/AA1100$ alloy composites reveals the clustering of ZrO_2 particles. The results obtained from the present work indicate that the normalized tensile strength and elastic modulus decrease with ZrO₂ particle clustering in AA1100 alloy matrix.

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