Numerical Investigation of the Effect of Particle Clustering on the Micromechanical Properties of Titanium Nitride/AA4015 Alloy Particle-Reinforced Metal Matrix Composites

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Abstract: *In the current work, the TiN/AA4015 metal matrix composites were fabricated at 10%, 20% and 30% volume fractions of TiN. These composites were analyzed with finite element analysis code with and without clustering of TiN particles. The microstructure of TiN/AA4015 alloy composites reveals the clustering of TiN particles. The tensile strength and elastic modulus decrease with clustering of TiN particles in AA4015 alloy matrix. To break clustering of the TiN particles in the metal matrix, the requirement of tensile strength is much high.*

Keywords: *AA4015, titanium nitride, spherical nanoparticle, RVE model, finite element analysis, clustering.*

1. INTRODUCTION

Particulate metal matrix composites have been shown to present improvements in strength, wear resistance, structural efficiency, reliability and control of physical properties such as density and coefficient of thermal expansion, thus providing improved engineering performance in contrast to the un-reinforced matrix. One of the major challenges when processing MMCs is achieving a homogeneous distribution of reinforcement in the matrix as it has a strong impact on the properties and the quality of the material [1]. The casting processing methods often produce agglomerated particles in the ductile matrix and as a result they exhibit extremely low ductility [2]. Clustering leads to a non-homogeneous response and lower macroscopic mechanical properties. Particle clusters act as crack or decohesion nucleation sites at stresses lower than the matrix yield strength, causing the MMC to fail at unpredictable low stress levels [3, 4]. Possible reasons resulting in particle clustering are chemical binding, surface energy reduction or particle segregation.

The aim of this paper is to evaluate the influence of particle clustering on micromechanical properties using the finite element method (FEM). The shape of titanium nitride nanoparticle considered in this work is spherical. The periodic particle distribution was a square array [5-18]. 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.

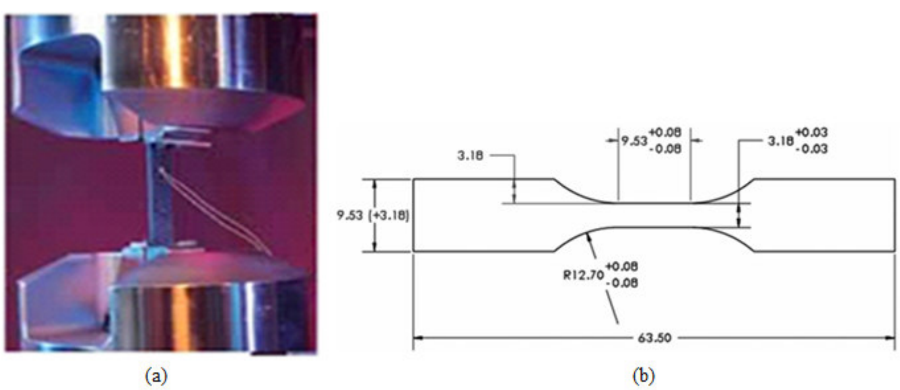

Figure 1: Tensile testing: UTM with temperature controlled chamber and (b) shape and dimensions of tensile specimen.

2. MATERIALS METHODS

The matrix material was AA4015 alloy. The reinforcement material was titanium nitride (TiN) nanoparticles of average size 100nm. TiN/AA4015 alloy composites were fabricated by the stir casting process and low pressure casting technique with 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 1) 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 TiN/AA4015 composites at three (10%, 20% and 30%) volume fractions of TiN. 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 TiN particles is shown in figure 2a and that with clustering of BN particles is shown in figure 2b.

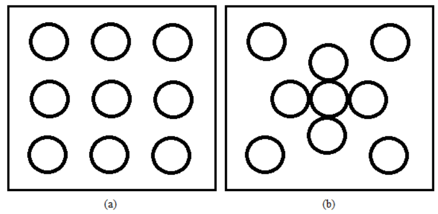

Figure 2: The interphase in a nanoparticle-reinforced composite: (a) without clustering and (b) with clustering.

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 [19, 20] is stated below:

$$\sigma_c = \left[\sigma_m \left\{\frac{1-(v_p+v_v)^{2/3}}{1-1.5(v_p+v_v)}\right\}\right] e^{m_p(v_p+v_v)} + kd_p^{-1/2} \quad (1)$$

$$k = E_m m_m / E_p m_p$$

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_m 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

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

The lower-bound equation is given by

$$\frac{E_c}{E_m} = 1 + \frac{v_p - v_p}{\delta/(\delta-1)-(v_p+v_v)^{1/3}} \quad (3)$$

where, $\delta = E_p / E_m$.

The transverse modulus is given by

$$E_t = \frac{E_m E_p}{E_m + E_p(1-v_p{}^{2/3})/v_p{}^{2/3}} + E_m\left(1 - v_p{}^{2/3} - v_v{}^{2/3}\right) \quad (4)$$

3. RESULTS AND DISCUSSION

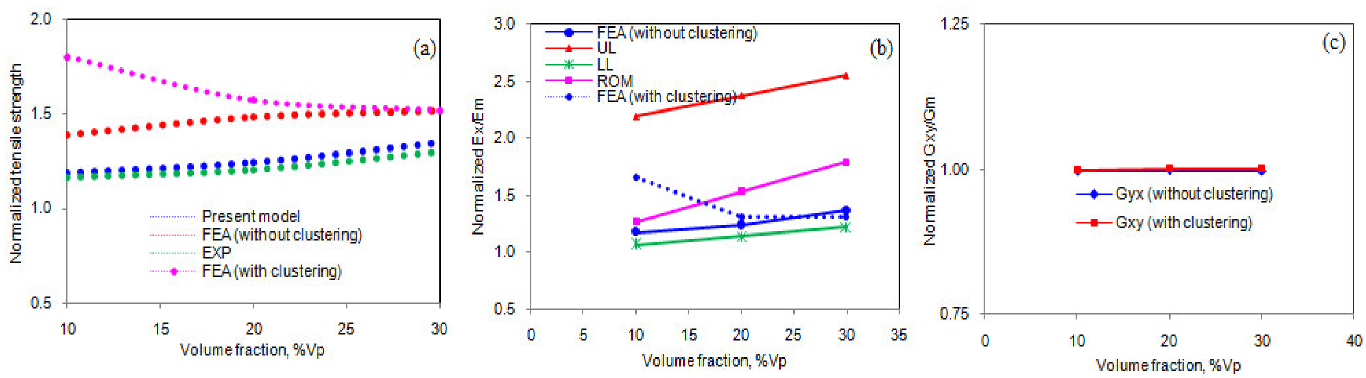

Figure 3: Effect of volume fraction on (a) normalized strength, (b) normalized tensile elastic modulus and (c) normalized shear modulus of TiN/AA4015 composites.

Figure 3a represents the normalized tensile stresses induced in the composites. The tensile stresses induced in the composites were normalized with tensile strength of AA4015 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 TiN particles, the tensile stress increases with increase of volume fraction of TiN in AA4015 alloy matrix. However, the tensile stress decreases in the case of clustering of TiN particles. The normalized elastic modulus increases with increase of volume fraction of non-clustered TiN particles in AA4015 alloy matrix; while it decreases with increase of volume fraction of clustered TiN particles in AA4015 alloy matrix (figure 3b). The normalized shear modulus is constant with increase of volume fraction of TiN with and without clustering of particles (figure 3c). The optical micrograph as shown in figure 4 reveals random distribution of 20%TiN and 30% TiN (30% Vp) particles in AA4015 alloy matrix. The clustering of particles is also seen in the microstructure illustrated in figure 4. In microstructures of TiN/AA4015 alloy composites, the reinforcement TiN particles have agglomerated forming clusters preferentially located at the grain boundaries or the interdendritic regions. This can be attributed to the pushing of the particles by the solidification front.

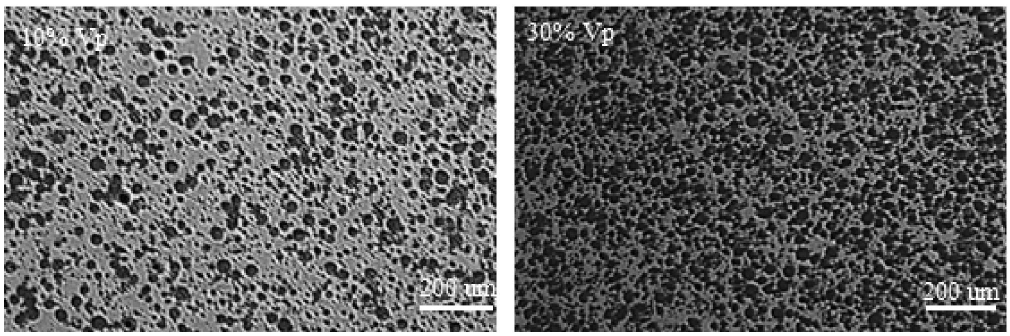

Figure 3: Microstructure showing distribution of 10% and 30% TiN nanoparticles in AA4015 alloy matrix.

Intensive shearing is required to break down the agglomerates into individual particles by applying a shear stress that will overcome the average cohesive force or the tensile strength of the cluster as observed 20% and 30% volume fractions with clustered TiN particles (figure 4). According to this, for a smaller particle size and shorter interparticle distance, which is the case for nanoparticles, the tensile strength is much higher making the application of a high shear stress important in order to break the clusters.

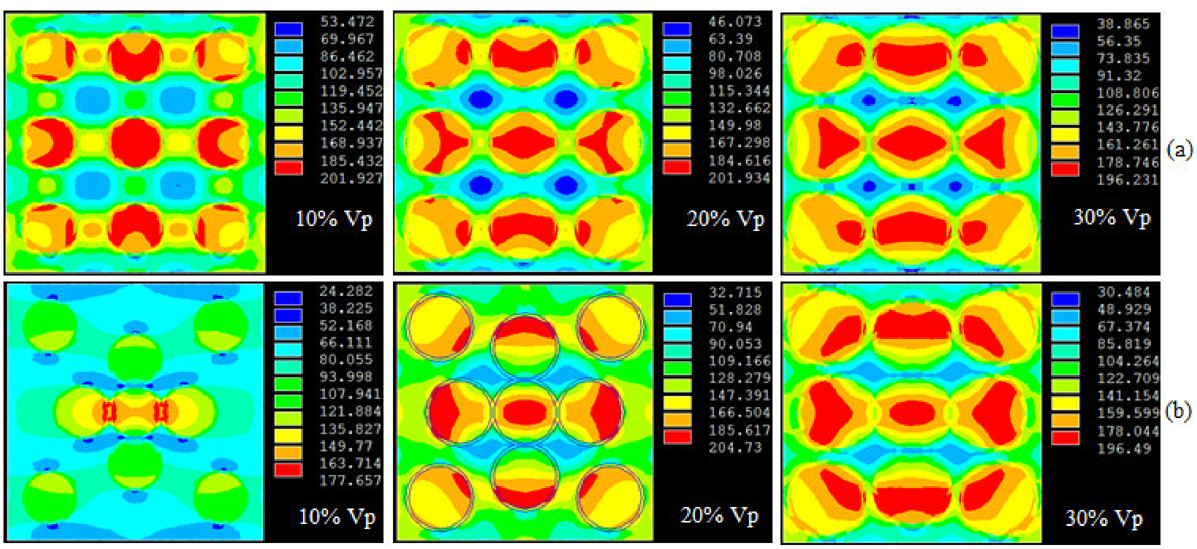

Figure 4: Images of von Mises stresses obtained from FEA: (a) without clustering and (b) with clustering.

4. CONCLUSION

TiN/AA4015 alloy composites were analyzed following two different schemes: (i) uniform distribution of TiN particles without clustering and (ii) clustering of TiN particles. For shorter interparticle distance due to clustering of the TiN particles in the metal matrix, the requirement of tensile strength is much high to break the clusters. The tensile stress, shear stress and elastic modulus decrease with the clustering of particles TiN/ AA4015 composites.

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