# Agglomeration of Nanoparticles into Network Aggregates in Zirconium Carbide/AA6061 Alloy Particle Reinforced Composites

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**Abstract:** *In the current work, the* ZrC / *AA6061 alloy metal matrix composites were fabricated at 10%, 20% and 30% volume fractions of* ZrC*. These composites were analyzed with finite element analysis code with and without clustering of* ZrC *particles. In the clustering regions, the stress induced was found to be high.. The tensile strength and elastic modulus decrease with clustering of* ZrC *particles in AA6061 alloy matrix.*

**Keywords:** *AA6061, zirconium carbide, spherical nanoparticle, unit-cell, finite element analysis, clustering.*

## 1. INTRODUCTION

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]. To obtain a specific mechanical/physical property, ideally, the MMC should consist of fine particles distributed uniformly in a ductile matrix and with clean interfaces between particle and matrix. However, the current processing methods often produce agglomerated particles in the ductile matrix and as a result they exhibit extremely low ductility. 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 [2]. Possible reasons resulting in particle clustering are chemical binding, surface energy reduction or particle segregation [3]. The agglomerative nature of ultrafine particles due to their high cohesive energy leads to an increase in the total surface area and increases their tendency to clump together forming agglomerates and clusters, inducing an unwanted brittle nature to metal matrix composites [4].

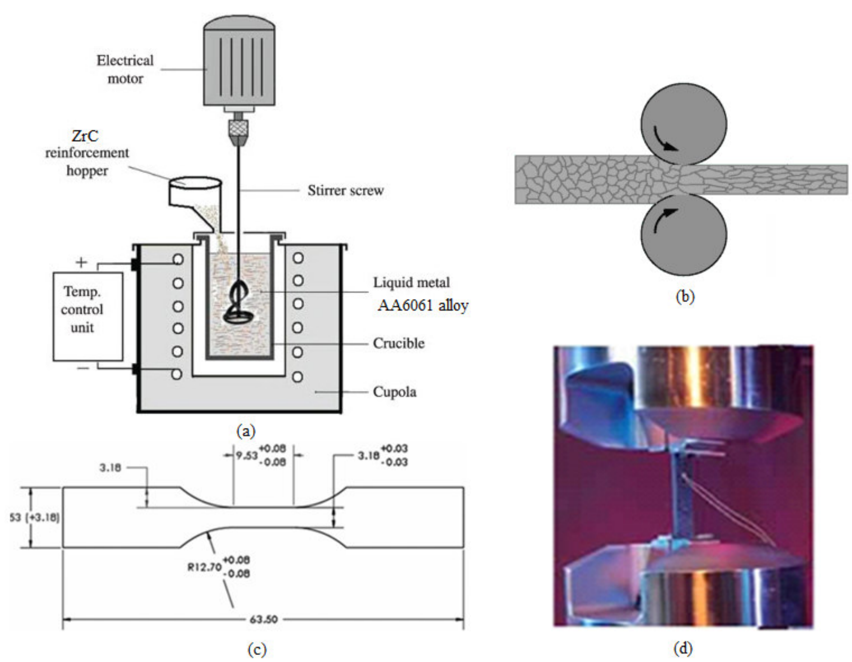


**Figure 1:** Stir casting process; cold rolling (b); shape and dimensions of tensile specimen (c); and tensile testing on UTM (d)

The objective of the present work was to estimate the effect of reinforcement clustering on the micromechanical behavior in zirconium carbide/AA6061 alloy metal matrix composites. A two-dimensional unit-cell model in the periodic boundary condition [5-18] was developed using finite element method (FEM) to analyze the stress distribution in the clustering and non-clustering regions. The shape of zirconium carbide (ZrC) nanoparticle considered in this work is spherical.

## 2. MATERIALS METHODS

The matrix material was AA6061 alloy. The reinforcement material was ZrC nanoparticles of average size 100nm. AA6061alloy/ZrC 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 ZrC /AA6061 composites at three (10%, 20% and 30%) volume fractions of ZrC. 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 ZrC particles is shown in figure 2a and that with clustering of ZrC particles is shown in figure 2b.

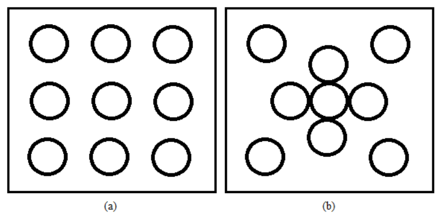


**Figure 2:** The interphase in a nanoparticle-reinforced composite: (a) without clustering and (b) with clustering.

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:

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

$$k = E_m m_m / E_p m_p$$

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

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

The lower-bound equation is given by

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

where, $\delta = E_p/E_m$ .

The transverse modulus is given by

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

## 3. RESULTS AND DISCUSSION

Figure 3a shows the variation of the strengths of the composites with the reinforcement concentrations. Adding the reinforcement to the matrix alloy led to the increased tensile strength without clustering ZrC particles. However, due to the effect of the reinforcement clusters the tensile strength decreases with increase of ZrC content in AA6061 alloy matrix. The tensile stresses obtained from the finite element analysis (FEA) are higher than those obtained from the mathematical expression mentioned in Eq.(1) and the experimental procedure as shown in figure 3a. The ZrC particles distributions in various composites are shown in figure 4. For the composite with a volume fraction of 10 vol.%, the ZrC particles were randomly distributed with less number of clusters. For the composites with higher reinforcement contents (≥ 20 vol.%), although the distributions of the ZrC particles were still relatively homogeneous, clusters began to appear. The normalized elastic modulus increases with increase of volume fraction of non-clustered ZrC particles in AA6061 alloy matrix; while it decreases with increase of volume fraction of clustered ZrC particles in AA6061 alloy matrix (figure 3b). The normalized shear modulus is constant with increase of volume fraction of ZrC without clustering of particles (figure 3c); whereas it decreases with increase of volume fraction of ZrC with clustering of particles. There is no much variation in the shear modulus for the volume fractions of 20% and 30% with clustered ZrC particles. This result seems to indicate that small variations in the degree of clustering.

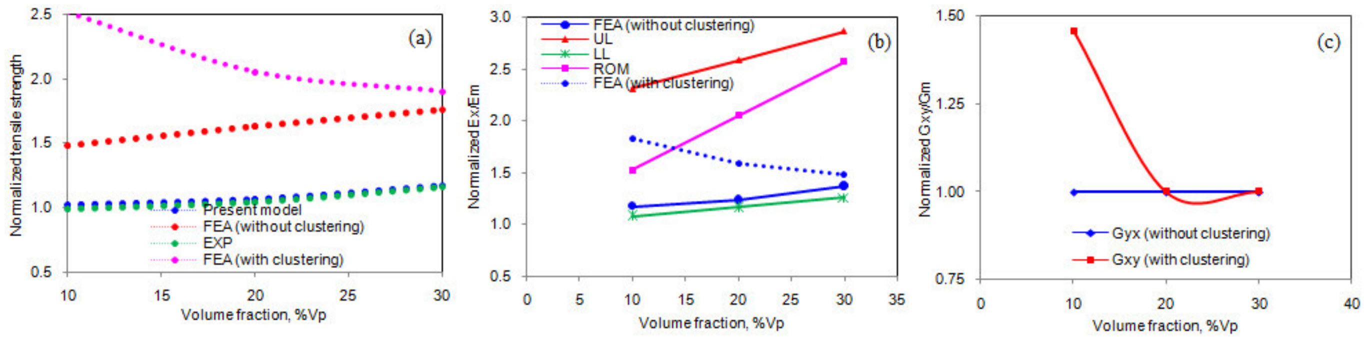


**Figure 3:** Effect of volume fraction on (a) normalized strength, (b) normalized tensile elastic modulus and (c) normalized shear modulus of ZrC/AA6061 composites.

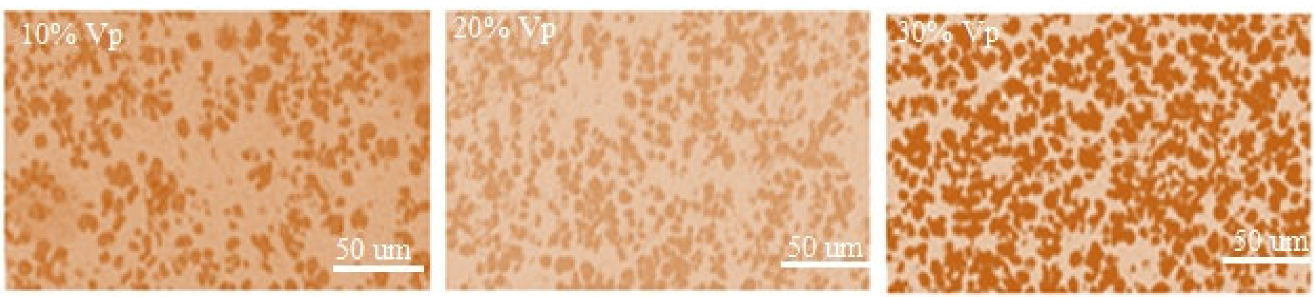


**Figure 3:** Microstructure showing distribution of 10%, 20% and 30% ZrC nanoparticles in AA6061 alloy matrix.

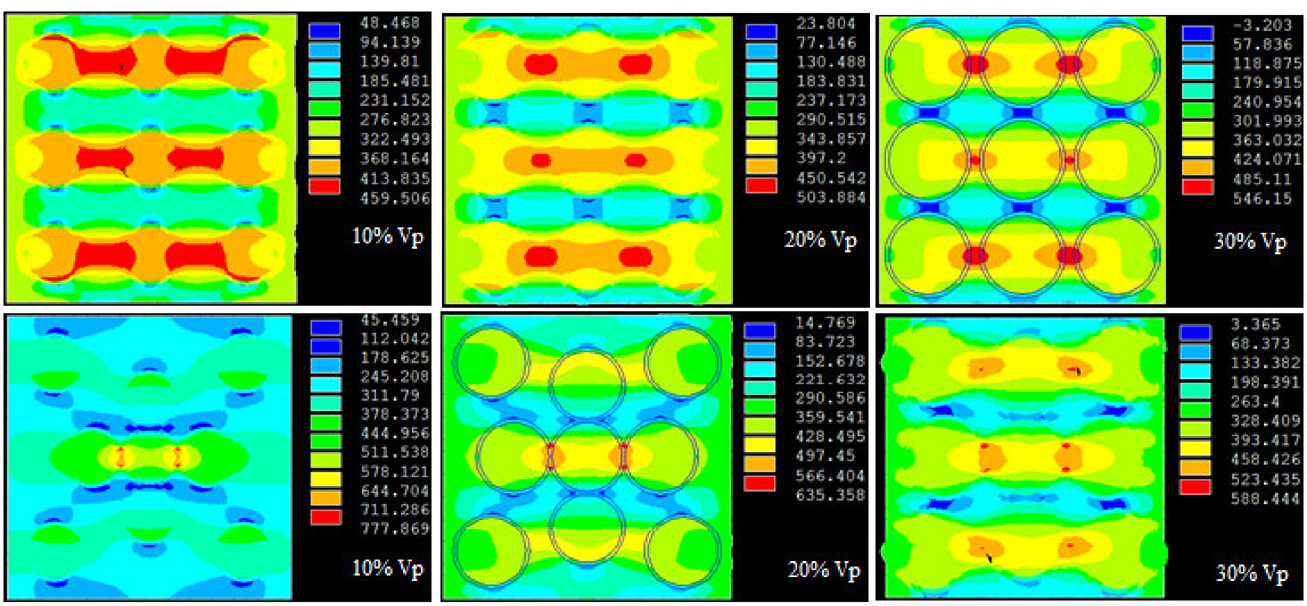


**Figure 4:** Images of tensile stresses obtained from FEA: (a) without clustering and (b) with clustering.

In all the models (figure 4), the ZrC particles-AA6061 alloy interface edges experience higher stresses. This is attributed to the fact of the stress concentration in the vicinity of the reinforcement.

## 4. CONCLUSION

ZrC/AA6061 alloy composites were analyzed following two different schemes: (i) uniform distribution of ZrC particles without clustering and (ii) clustering of ZrC particles. The stresses developed in the clustering regions are higher than those developed in other sides of the clustering regions. The tensile stress, shear stress and elastic modulus decrease with the clustering of particles ZrC/AA6061 composites.

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