Effects of Adhesive and Interphase Characteristics between Matrix and Reinforced Nanoparticle of AA7175/AlN Nanocomposites

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Abstract: ***Theoretical models were unable to examine the overall elastic-plastic response during the deformation of metal matrix composites. On the other hand, numerical micromechanical modeling analysis appears to be well-suited to describe the behavior of these composites. In this article two types of RVE models have been implemented using finite element analysis. Aluminum nitride nanoparticles were used as a reinforcing material in the matrix of AA7175 aluminum alloy. It has been observed that the nanoparticle did not overload during the transfer of load from the matrix to the nanoparticle via the interphase due to interphase between the nanoparticle and the matrix. Due to interphase between the nanoparticle and the matrix, the tensile strength increases from 510.60 to 532.51 MPa.***

Keywords: RVE models, AlN, AA7175, finite element analysis, interphase.

1. Introduction

Metal matrix composites (MMCs) have been increased attention in recent years resulting from the need for materials with high strength and stiffness in the fields for a large number of functional and structural applications. The higher stiffness of ceramic particles can result in an incremental increase in the stiffness of a composite [1, 2]. One of the major challenges when processing nanocomposites 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. The current processing methods often generate agglomerated particles in the ductile matrix and as a result they exhibit extremely low ductility [3]. Particle clusters act as crack or decohesion nucleation sites at stresses lower than the matrix yield strength, causing the nanocomposite to fail at unpredictable low stress levels. Possible reasons resulting in particle clustering are chemical binding, surface energy reduction or particle segregation [4-6]. While manufacturing Al alloy-AlN nanocomposites, the wettability factor is the main concern irrespective of the manufacturing method. Its superior surface activity restricts its incorporation in the metal matrix. One of the methods consists of adding surfactant which serves as a wetting agent in molten metal to enhance wettability of particulates. Researchers have successfully used several surfactants like Li, Mg, Ca, Zr, Ti, Cu, and Si for the synthesis of nanocomposites [7-9].

The objective of this article was to develop AA7175/AlN nanocomposites with and without interphase between AlN nanoparticle and AA7175 matrix. The RVE models were used to analyze the nanocomposites using finite element analysis. A homogeneous interphase region was assumed in the models.

2. Theoretical Background

Analyzing structures on a microstructural level, however, are clearly an inflexible problem. Analysis methods have thus sought to approximate composite structural mechanics by analyzing a representative section of the composite microstructure, commonly called a Representative Volume Element (RVE). One of the first formal definitions of the RVE was given by Hill [10] who stated that the RVE was (1) structurally entirely typical of the composite material on average and (2) contained a sufficient number of inclusions such that the apparent moduli were independent of the RVE boundary displacements or tractions. Under axisymmetric as well as antisymmetric loading, a 2-D axisymmetric model can be used for the cylindrical RVE, which can significantly reduce the computational work [11].

To derive the formulae for deriving the equivalent material constants, a homogenized elasticity model of the square representative volume element (RVE) as shown in figure 1 is considered. The dimensions of three-dimensional RVE are 2a x 2a x 2a. The cross-sectional area of the RVE is 2a x 2a. The elasticity model is filled with a single, transversely isotropic material that has five independent material constants (elastic moduli E_y and E_z, Poison's ratios v_{xy}, v_{yz} and shear modulus G_{yz}). The general strain-stress relations relating the normal stresses and the normal stains are given below:

$$\varepsilon_x = \frac{\sigma_x}{E_x} - \frac{v_{xy}\sigma_y}{E_y} - \frac{v_{xz}\sigma_z}{E_z} \quad (1)$$

$$\varepsilon_y = -\frac{v_{yx}\sigma_x}{E_y} + \frac{\sigma_y}{E_y} - \frac{v_{yz}\sigma_z}{E_z} \quad (2)$$

$$\varepsilon_z = -\frac{v_{zx}\sigma_x}{E_x} - \frac{v_{zy}\sigma_y}{E_y} + \frac{\sigma_z}{E_z} \quad (3)$$

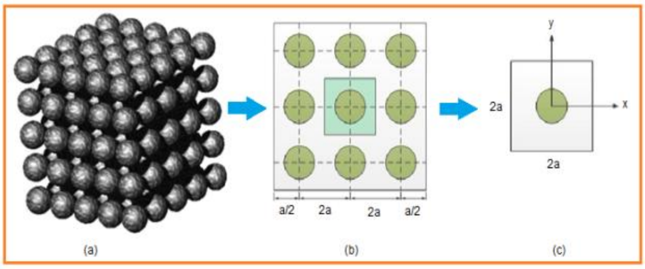

Figure1: A square RVE containing a nanoparticle.

Let assume that $\sigma_{xy} = \sigma_{yx}$, $\sigma_{yz} = \sigma_{zy}$ and $\sigma_{zx} = \sigma_{xz}$. For plane strain conditions, $\epsilon_z = 0$, $\epsilon_{yz} = \varepsilon_{zx} = 0$ and $\sigma_{yz} = \sigma_{zx}$. The above equations are rewritten as follows:

$$\varepsilon_x = \frac{\sigma_x}{E_x} - \frac{v_{xy}\sigma_y}{E_y} - \frac{v_{yz}\sigma_z}{E_z} \quad (4)$$

$$\varepsilon_y = -\frac{v_{xy}\sigma_x}{E_y} + \frac{\sigma_y}{E_y} - \frac{v_{yz}\sigma_z}{E_z} \quad (5)$$

$$\varepsilon_z = -\frac{v_{yz}\sigma_x}{E_z} - \frac{v_{yz}\sigma_y}{E_z} + \frac{\sigma_z}{E_z} \quad (6)$$

To determine E_y and E_z, v_{xy} and v_{yz}, four equations are required. Two loading cases as shown in figure 22 have been designed to give four such equations based on the theory of elasticity. For load case (figure 2a), the stress and strain components on the lateral surface are:

$$\sigma_x = \sigma_y = 0$$

$$\varepsilon_x = \frac{\Delta a}{a} \text{ along } x = \pm a \text{ and } \varepsilon_y = \frac{\Delta a}{a} \text{ along } y = \pm a$$

$$\varepsilon_z = \frac{\Delta a}{a}$$

where Δa is the change of dimension a of cross-section under the stretch Δa in the z-direction. Integrating and averaging Eq. (6) on the plane z = a, the following equation can be arrived:

$$E_z = \frac{\sigma_{ave}}{\varepsilon_z} = \frac{a}{\Delta a}\sigma_{ave} \quad (7)$$

where the average value of σ_z is given by:

$$\sigma_{ave} = \iint \sigma_z\,(x, y, a)\,dxdy \quad (8)$$

The value of σ_{ave} is evaluated for the RVE using finite element analysis (FEA) results.

Using Eq. (5) and the result (7), the strain along $y = \pm a$:

$$\varepsilon_y = -\frac{v_{yz}\sigma_z}{E_z} = -v_{yz}\frac{\Delta a}{a} = \frac{\Delta a}{a}$$

Hence, the expression for the Poisson's ratio v_{yz} is as follows:

$$v_{yz} = -1 \quad (9)$$

For load case (figure 2b), the square representative volume element (RVE) is loaded with a uniformly distributed load (negative pressure), P in a lateral direction, for instance, the x-direction. The RVE is constrained in the z-direction so that the plane strain condition is sustained to simulate the interactions of RVE with surrounding materials in the z-direction. Since, $\varepsilon_z = 0$, $\sigma_z = v_{yz}(\sigma_x + \sigma_y)$ for the plain stress, the strain-stress relations can be reduced as follows:

$$\varepsilon_x = \left(\frac{1}{E_x} - \frac{1}{E_z}\right)\sigma_x - \left(\frac{v_{xy}}{E_y} + \frac{1}{E_z}\right)\sigma_y \quad (10)$$

$$\varepsilon_y = -\left(\frac{v_{xy}}{E_x} + \frac{1}{E_z}\right)\sigma_x + \left(\frac{1}{E_x} - \frac{1}{E_z}\right)\sigma_y \quad (11)$$

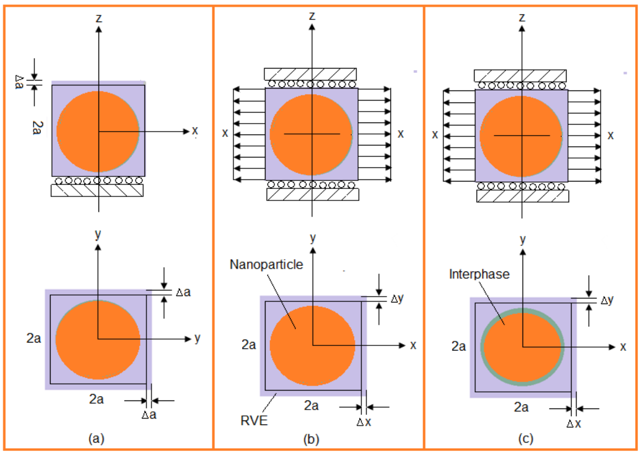

Figure 2: RVE models

For the elasticity model as shown in figure 2b, one can have the following results for the normal stress and strain components at a point on the lateral surface:

$$\sigma_y = 0,\ \sigma_x = P$$

$$\varepsilon_x = \frac{\Delta x}{a} \text{ along } x = \pm a \text{ and } \varepsilon_y = \frac{\Delta y}{a} \text{ along } y = \pm a$$

where Δx (>0) and Δy (<0) are the changes of dimensions in the x- and y- direction, respectively for the load case shown in Fig.2b. Applying Eq. (11) for points along $y = \pm a$ and Eq. (10) for points along $x = \pm a$, we get the following:

$$\varepsilon_y = -\left(\frac{v_{xy}}{E_x} + \frac{1}{E_z}\right)P = \frac{\Delta y}{a} \quad (12)$$

$$\varepsilon_x = \left(\frac{1}{E_x} - \frac{1}{E_z}\right)P = \frac{\Delta x}{a} \quad (13)$$

By solving Eqs. (12) and (13), the effective elastic modulus and Poisson's ratio in the transverse direction (xy-plane) as follows:

$$E_x = E_y = \frac{1}{\frac{\Delta x}{Pa} + \frac{1}{E_z}} \quad (14)$$

$$v_{xy} = \left(\frac{\Delta y}{Pa} + \frac{1}{E_z}\right) / \left(\frac{\Delta x}{Pa} + \frac{1}{E_z}\right) \quad (15)$$

In which E_z can be determined from Eq. (7). Once the change in lengths along x- and y- direction (Δx and Δy) are determined for the square RVE from the FEA, E_y (= E_x) and v_{xy} can be determined from Eqs. (14) and (15), correspondingly.

The young's modulus of the interphase is obtained by the following formula:

$$E_i(r) = (\alpha E_p - E_m)\left(\frac{r_i - r}{r_i - r_p}\right) + E_m \quad (16)$$

3. Materials Methods

The matrix material was AA7175 aluminum alloy. AA7175 contains Si (12.50%), Cr (≤0.10%), Cu (1.20%), Fe (≤1.00%), Mg (1.10%), Ni (1.00%) and Zn (≤0.25%) as its major alloying elements. The reinforcement material was aluminum nitride (AlN) nanoparticles of average size 100nm. The mechanical properties of materials used in the present work are given in table 1.

Table 1: Mechanical properties of AA7175 matrix and AlN nanoparticles

Property	AA7175	AlN
Density, g/cc	2.68	3.26
Elastic modulus, GPa	78.6	330
Ultimate tensile strength, MPa	379	270
Poisson's ratio	0.33	0.24

In this research, a cubical RVE was implemented to analyze the tensile behavior AA7175/AlN nanocomposites (Fig.2c). The determination of the RVE's dimensional conditions requires the establishment of a volumetric fraction of spherical nanoparticles in the composite. Hence, the weight fractions of the particles were converted to volume fractions. The volume fraction of a particle in the RVE ($V_{p,rve}$) is determined using Eq.(17):

$$v_{p,rve} = \frac{\text{Volume of nanoparticle}}{\text{Volume of RVE}} = \frac{16}{3} \times \left(\frac{r}{a}\right)^3 \quad (17)$$

where, r represents the particle radius and a indicates the diameter of the cylindrical RVE. The volume fraction of the particles in the composite (V_p) is obtained using equation

$$V_p = (w_p/\rho_p)/(w_p/\rho_p + w_m/\rho_m) \quad (18)$$

where ρ_m and ρ_p denote the matrix and particle densities, and w_m and w_p indicate the matrix and particle weight fractions, respectively.

The RVE dimension (a) was determined by equalizing Eqs. (17) and (18). Two RVE schemes namely: without interphase (adhesion) and with interphase were applied between the matrix and the filler. The loading on the RVE was defined as symmetric displacement, which provided equal displacements at both ends of the RVE. To obtain the nanocomposite modulus and yield strength, the force reaction was defined against displacement. The large strain PLANE183 element [12] was used in the matrix and the interphase regions in all the models. In order to model the adhesion between the interphase and the particle, a COMBIN14 spring-damper element was used. The stiffness of this element was taken as unity for perfect adhesion which could determine the interfacial strength for the interface region.

It is equally important to set the strain rates of the finite element models based on the experimental tensile tests' setups to converge an exact nonlinear solution. Hence, FEM models of different RVEs with various particle contents should have comparable error values. In this respect, the ratio of the tensile test speed/the gauge length of the specimens should be the same as the corresponding ratio in the RVE displacement model. Therefore, the rate of displacement in the RVEs was set to be 0.1 (1/min).

4. Results and Discussion

The AlN/AA7175 nanocomposites with or without interphase were modeled using finite element analysis (ANSYS) to analyze the tensile behavior and fracture.

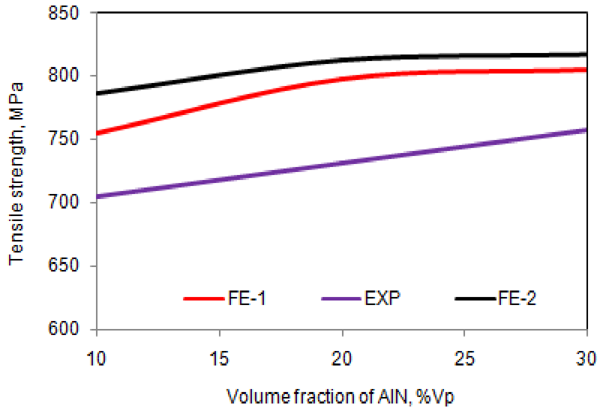

Figure 3: Effect of volume fraction on tensile strength along tensile load direction

4.1 Tensile behavior

An increase of AlN content in the matrix could increase the tensile strength of the nanocomposite (figure 3). The maximum difference between the FEA results without interphase and the experimental results was 66.89 MPa. This differentiation can be attributed to lack of bonding between the AlN nanoparticle and the AA7175 matrix. The maximum difference between the FEA results with interphase and the experiments results was 81.36 MPa. This discrepancy can be endorsed to the presence of voids in the nanocomposites.

For 10%, 20% and 30%Vp of AlN in AA7175, without interphase and barely consideration of adhesive bonding between the AlN nanoparticle and the AA7175 matrix, the loads transferred from the AlN nanoparticle to the AA7175 matrix were, respectively, 122.65 MPa, 192.58 MPa and 196.64 MPa (figure 4a) along the tensile load direction. Similarly, for 10%, 20% and 30%Vp of AlN in AA7175, with interphase and wetting between the ALN nanoparticle and the AA7175 matrix, the loads transferred from the AlN nanoparticle to the AA7175 matrix were, respectively,184.12 MPa, 252.66 MPa and 201.60 MPa (figure 4b) along the tensile load direction. Zhengang et al [13] carried a study improving wettability by adding Mg as the wetting agent. They suggested that the wettability between molten Al-Mg matrix and SiC particles is improved and the surface tension of molten Al-Mg alloy with SiC particle is reduced, and results in homogeneous particles distribution and high interfacial bond strength. For instance, addition of Mg to composite matrix lead to the formation of MgO and $MgAl_2O_3$ at the interface and this enhances the wettability and the strength of the composite [14].

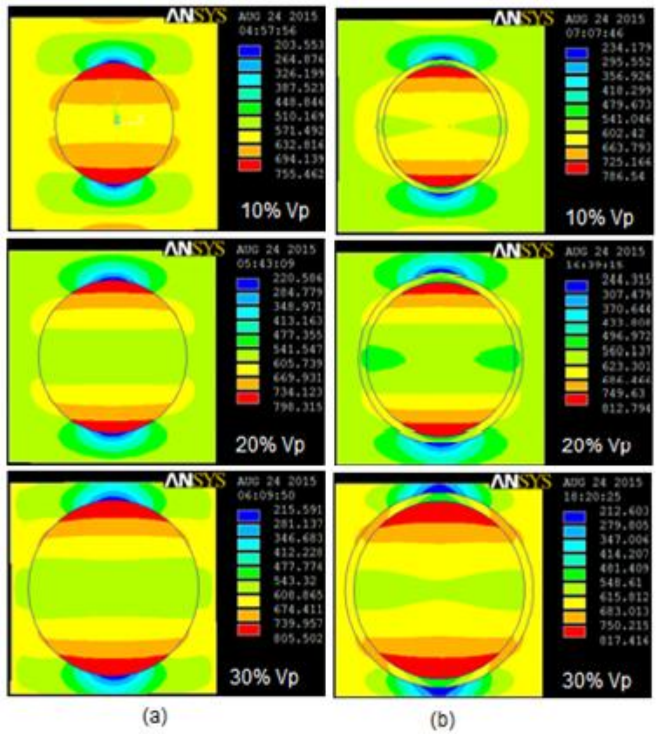

Figure 4: Tensile stresses (a) without interphase and (b) with interphase normal to load direction.

4.2 Fracture behavior

Figure 5 depicts the increase of von Mises stress with increase of volume fraction of AlN. In the case of nanocomposites with interphase between the nanoparticle and the matrix, the stress was transferred through shear from the matrix to the particles resulting low stress in the matrix. The stress transfer from the matrix to the nanoparticle was less for the nanocomposites without interphase resulting high stress in the matrix. Landis and McMeeking [15] assume that the fibers carry the entire axial load, and the matrix material only transmits shear between the fibers. Based on these assumptions alone, it is generally accepted that these methods will be most accurate when the fiber volume fraction V_f and the fiber-to matrix moduli ratio E_f / E_m are high. In the present case, the elastic moduli of AA7175 matrix and AlN nano particle are, respectively, 72.0 GPa and 330 GPa.

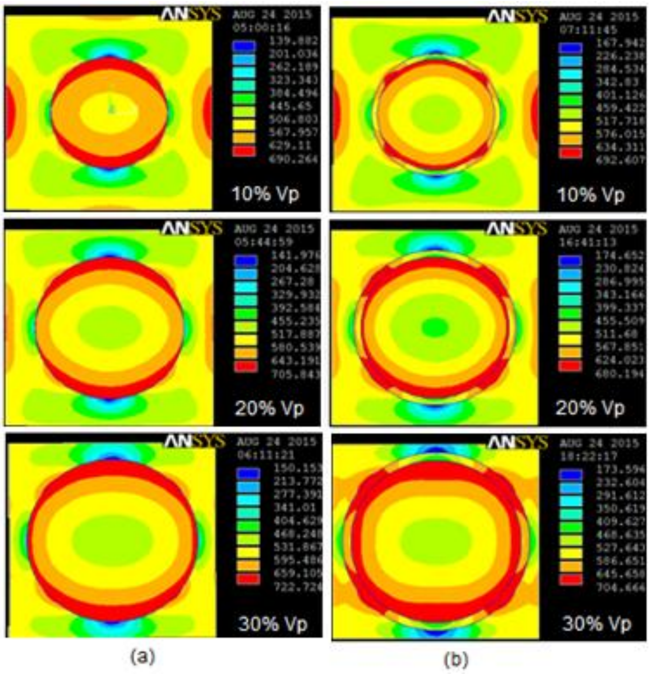

Figure 5: von Mises stress (a) and shear stress (b).

5. Conclusion

The RVE models give the trend of phenomenon happening in the nanocomposites. Without interphase and barely consideration of adhesive bonding, the tensile strength has been found to be 805.50 MPa for the nanocomposites consisting of 30%Aln nanoparticles. Due to interphase between the nanoparticle and the matrix, the tensile strength increases to 817.42 MPa. The tensile strengths obtained by author's model (with voids) are in good agreement with the experimental results. In the case of nanocomposites with interphase between the nanoparticle and the matrix, the stress is transferred through shear from the matrix to the particles. The transverse moduli of AlN/AA7175 nanocomposites have been found to be 20.64 GPa and 26.47 GPa, respectively, without and with interphase.

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