Two dimensional (2D) RVE-Based Modeling of Interphase Separation and Particle Fracture in Graphite/5050 Particle Reinforced Composites

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Abstract: In the current work, the Gr/AA5050 alloy metal matrix composites were subjected to mechanical and thermal loads. The results obtained from the finite element analysis of Gr/AA5050 alloy composites reveal the interphase separation from the particle and the matrix. Also, the particle fracture has been detected in Gr/AA5050 composites.

Keywords: Graphite, AA5050 alloy, RVE model, finite element analysis, interphase separation, particle fracture.

1. INTRODUCTION

Metal matrix composites containing particles with a small aspect ratio of 1 have been studied extensively because of their technological and scientific importance. Many studies have been conducted on the mechanical properties of these particulate-filled metal matrix composites. Stiffness or Young's modulus can be readily improved by adding either micro- or nano-particles since rigid particles generally have a much higher stiffness than metal matrices [1]. However, strength strongly depends on the stress transfer between the particles and the matrix. For well-bonded particles, the applied stress can be effectively transferred to the particles from the matrix [25]; this clearly improves the strength [2]. However, for poorly bonded micro-particles, strength reductions occur by adding particles [3]. The mechanical properties of particulate–polymer composites depend strongly on the particle size, particle–matrix interface adhesion and particle loading. The interface plays a crucial role in the load transfer between the matrix and the reinforcement, very critically as well as dislocation-particle interactions, which are significant in strengthening and stiffening the composite. Moreover, the physical properties such as thermal conductivity, coefficient of thermal expansion (CTE), dimensional stability, etc are also closely related with the nature of the interface. Strengthening by the reinforcing phase in MMCs is critically dependent on the strength of the bond between matrix and reinforcement. Interfacial bonding can be categorized as mechanical and chemical [4]. Mechanical bonding is significant only in the case of fiber reinforced composites, when fibers have rough or faceted surfaces. Chemical bonding is important for all kinds of reinforcements, viz. fibers, whiskers and particulates. In multiphase materials, numerical modeling techniques, such as finite element method (FEM), are often more effective than analytical modeling. Another advantage of numerical modeling is that deformation and damage characteristics, particularly on a local scale, can be revealed. Numerical modeling of the behavior of multiphase materials has typically been conducted by assuming a single fiber, whisker, or particle of simple geometry in a unit cell model [5-18].

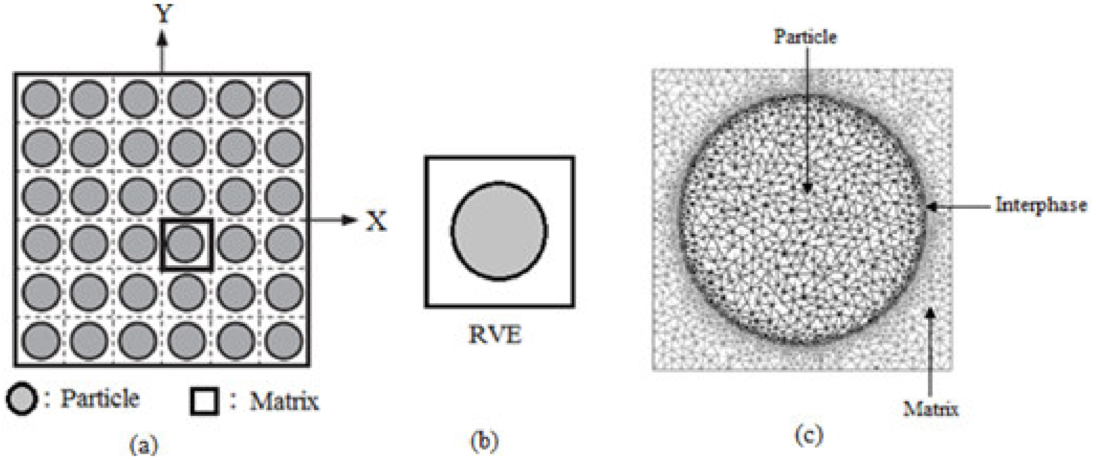

Figure 1: Square array of particles (a); Representative Volume Element (b); and Discretization of RVE (c).

The current work presents a finite element method capable of capturing the influence of volume fraction of graphite particles and thermo-mechanical loading on interphase separation and particle fracture. The shape graphite nanoparticle considered in this work is spherical. The periodic particle distribution was a square array and corresponding representative volume element (RVE) is showed in figure 1.

2. MATERIALS METHODS

The matrix material was AA5050 alloy. The reinforcement material was graphite (Gr) nanoparticles of average size 100nm. The mechanical properties of materials used in the present work are given in table 1. In the current work, a cubical representative volume element (RVE) was implemented to analyze the tensile behavior Gr/AA5050 alloy composites at two (10% and 30%) volume fractions of Gr 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.

Table 1: Mechanical properties of AA5050 matrix and Gr nanoparticles

Property	AA5050	Gr
Density, g/cc	2.69	2.51
Elastic modulus, GPa	68.9	445.0
Coefficient of thermal expansion, 10^{-6} 1/^{o}C	21.8	5.6
Specific heat capacity, J/kg/^{o}C	900	1288
Thermal conductivity, W/m/^{o}C	193	90
Poisson's ratio	0.33	0.19

3. RESULTS AND DISCUSSION

The normalized elastic moduli of Gr/AA5050 composites at different temperatures are shown in figure 2. The elastic moduli are normalized with the elastic modulus (E_m) of AA5050 alloy. The normalized elastic moduli, E_x/E_m and E_y/E_m, are decreased as shown in figure 2a. As the volume fraction of Gr increases the stiffness of the decreases when subjected thermo-mechanical loading. The normalized stiffness along the normal direction is lower than that along the load direction owing to tensile loading consideration in the present work. The normalized shear modulus increases with increase of temperature as shown in figure 2b. The increase of major Poisson's ratio with temperature indicates the elongation along the load is greater than that along the transverse direction of loading of RVE (figure 4c). However, the decrease of major ratio at 100^{o}C is not clear.

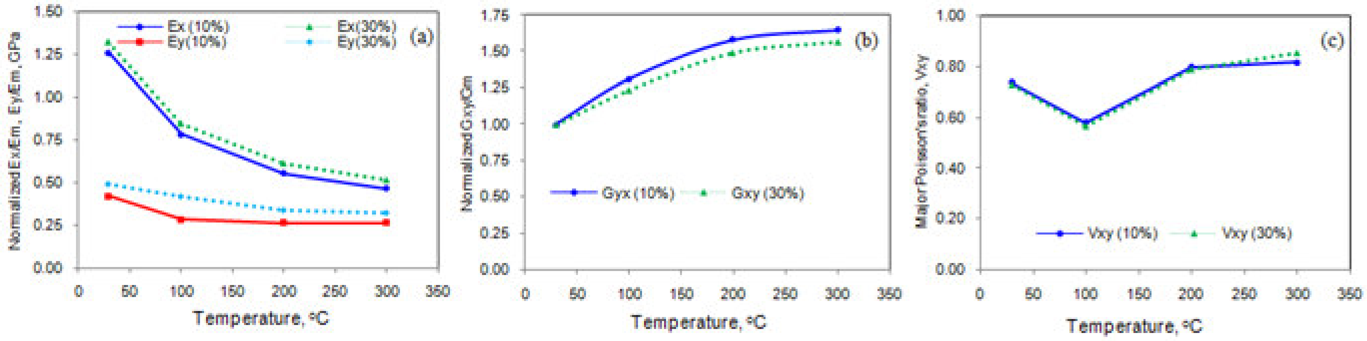

Figure 2: Effect of temperature on micromechanical properties of Gr/AA5050 composites.

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

$$\tau = \frac{n}{2}\sigma_p \qquad (1)$$

where σ_p is the particle stress. For the interfacial debonding/yielding to occur, the interfacial shear stress reaches its shear strength:

$$\tau = \tau_{max} \qquad (2)$$

For particle/matrix interfacial debonding can occur if the following condition is satisfied:

$$\tau_{max} < \frac{n\sigma_p}{2} \qquad (3)$$

It is observed from figure 3a that the interphase separation occurs between Gr nanoparticle and AA5050 alloy matrix as the condition in Eq.(3) is satisfied below 150^{o}C in 10% Gr/AA5050 composites while the interphase separation occurs 100^{o}C in 30% Gr/AA5050 composites. The normal displacement field (figure 4) across the interphase increases with increase of temperature. This confirms the increase of interphase separation from Gr particle and AA5050 alloy matrix with increase of temperature. Further, the normal and tangential tractions (figure 5) along the interphase increase with increase of temperature. If particle fracture occurs when the stress in the particle reaches its ultimate tensile strength, $\sigma_{p,uts}$, then setting the boundary condition at

$$\sigma_p = \sigma_{p,\ uts} \tag{4}$$

The relationship between the strength of the particle and the interfacial shear stress is such that if

$$\sigma_{P,uts} < \frac{2\tau}{n} \tag{5}$$

Then the particle will fracture. From the figure 3b, it is observed that the Gr nanoparticle was fractured above 150^{0}C in 10% Gr/AA5050 composites and above 75°C in 30% Gr/AA5050 composites only as the condition in Eq. (5) is satisfied.

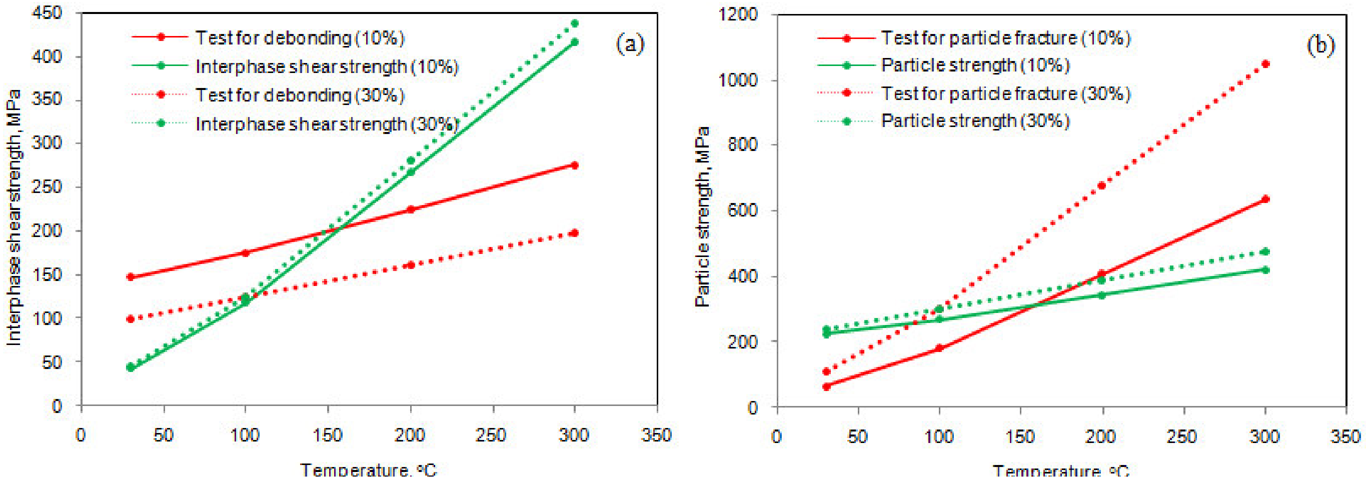

Figure 3: Criterion for interfacial debonding (a) and for particle fracture (b).

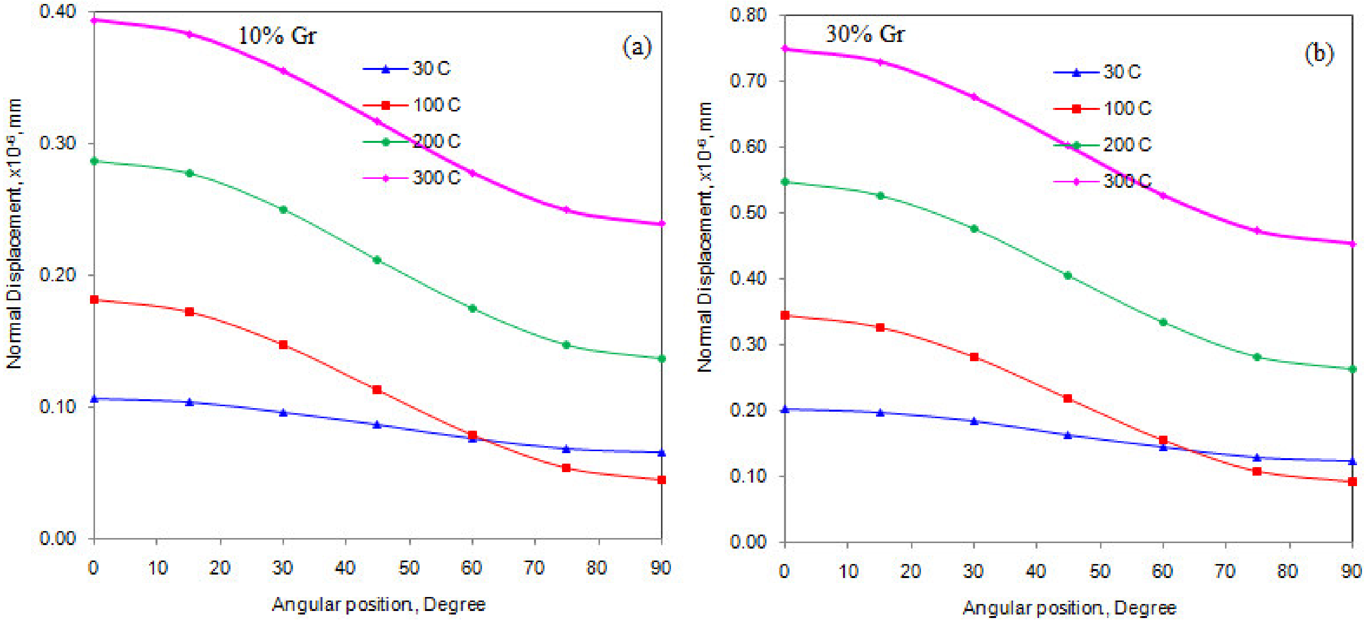

Figure 4: Normal displacement across the interphase between Gr particle and AA5050 alloy matrix.

The von Mises stress as a function of temperature is illustrated in figure 6. The von Mises stresses induced at the interface are higher than that induced in the nanoparticle. Hence, the interphase separation has occurred between the particle and the matrix. The particle fracture was also occurred in Gr/AA5050 alloy composites due to thermal shock.

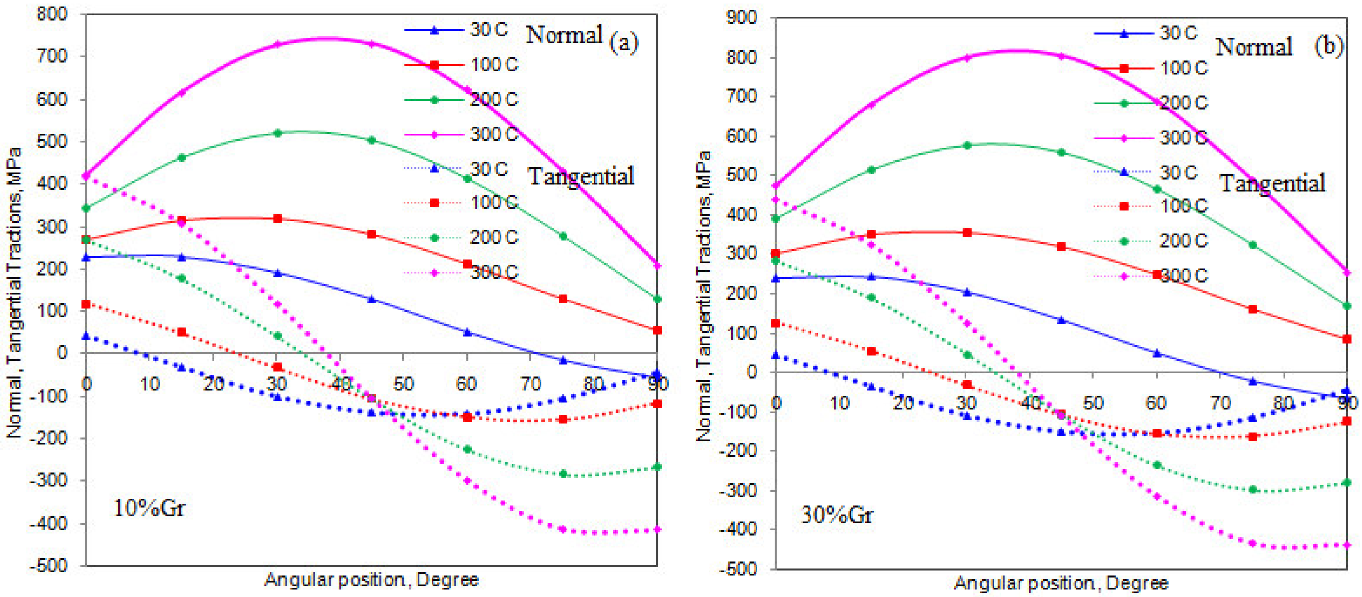

Figure 5: Normal and tangential tractions along the interphase.

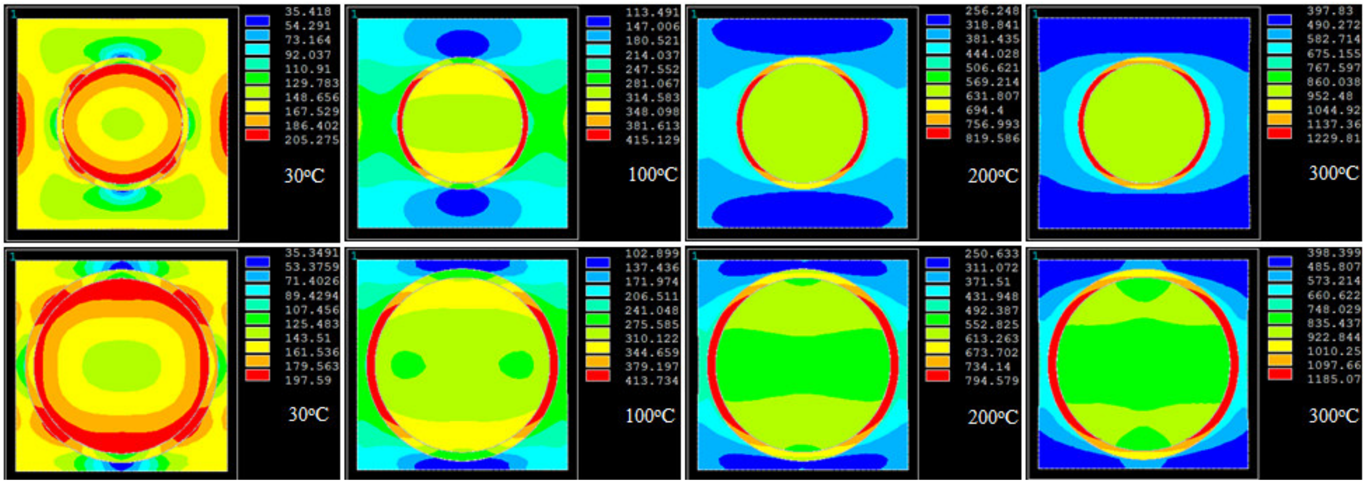

Figure 6: Images of von Mises stresses obtained from FEA: (a) 10% Gr/AA5050 alloy and (b) 30% Gr/AA5050 alloy composites.

4. CONCLUSION

The shear stress is high at the interface resulting to interphase separation from the particle and the matrix. The interphase separation has occurred between the particle and the matrix. The particle fracture has also occurred in Gr/AA5050 composites.

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