Influence of CTE Mismatch on Debonding and Particulate Damage in AA1100 Alloy/ZrC Nanoparticulate Metal Matrix Composites

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ABSTRACT: The aim of the present work was to predict the interface debonding and ZrC nanoparticulate fracture using RVE models through finite element analysis. The RVE model was designed from the square nanoparticulate distribution. The plane strain condition was assumed for 2-dimensional analysis of the composites. The major conclusion is that the ZrC nanoparticulates fracture above $100^{\circ}C$.

KEYWORDS: Zirconium carbide, AA1100 alloy, Particulate fracture, interface debonding, RVE model, finite element analysis.

I. INTRODUCTION

Nanoparticulate reinforced metal matrix composites are of great concern for several industrial applications due to their higher stiffness and strength than the alloys used for the matrix [1, 2]. Deep understanding of thermoplastic behaviour of the nanoparticulate reinforced metal matrix composites is an important subject in boosting up of those materials. The mismatch in coefficient of thermal expansion (CTE) and thermal conductivity between the nanoparticles and matrix can induce large stresses within the inclusions or at the matrix–nanoparticle interfaces. Several reinforcing materials nanoparticulates such as silicon carbide [3-7], alumina [8-10], boron carbide [11, 12], titanium boride [13, 14], silicon nitride [15-17], alumina trihydrate [18], carbon [19], etc were tested to improve the strength and stiffness.

The present work was to investigate the influence of CTE mismatch on interface debonding and particulate fracture in AA1100 alloy/ZrC nanoparticulate metal matrix composites. Finite element analysis (FEA) was executed using representative volume element (RVE) subjected to hydrostatic and isothermal loading.

II. MATERIAL AND METHODS

The shear lag model [20] has been used to describe the build up and transfer of particle stress, σ_p from the point where the particle enters the matrix to some point along the particle axis where the tensile stress has decayed to zero. Failure of the particle/matrix interface occurs when the interfacial shear strength, τmax, is reached.

The shear lag distribution of strain, along a fully bonded particle can be described by [20]

$$e_{app} = e_p \frac{sibh[n(L_{e-x/r})]}{sinH(ns)} \tag{1}$$

where e_{app} is the strain acting on the particle outside the matrix, e_p is the particle strain at a distance x inside the matrix, Le is the embedded length, r is the particle radius and s is the particle aspect ratio (L_e/r). The n parameter used in this paper is based on the parameter [14-16]:

$$n^2 = \frac{2}{E_p E_m}\left[\frac{E_p V_p + E_m V_m}{V_m/(4G_p) + 1/(2G_m)\left((1/V_m)\ln(1/V_p) - 1 - (V_m/2)\right)}\right] \tag{2}$$

where E_p and G_P ate the particle elastic and shear moduli, E_m and G_m are the elastic and shear moduli of the matrix. V_p is the particle volume fraction and V_m is the volume fraction of matrix. The corresponding interfacial stress, τ at a distance x along the interface, is given by

$$\tau = \frac{n}{2}E_p e_{app} \frac{\cosh[n(L_e-x)/r]}{\sinh[ns]} \tag{3}$$

Is a maximum at the crack plane (x = 0). Since both the interfacial shear stress and the stress acting on the particle, are a maximum at the crack-plane then failure should be expected to initiate from this point. When x = 0, the Eq. (3) becomes:

$$\tau = \frac{n}{2}E_p e_p \tag{4}$$

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

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

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

$$\sigma_p = \sigma_{p,uts} \tag{6}$$

and substituting into Eq.(5) gives a relationship between the strength of the particle and the interfacial shear stress such that if

$$\sigma_{P,uts} < \frac{2\tau}{n} \tag{7}$$

Then the particle will fracture. Similarly if interfacial debonding/yielding is considered to occur when the interfacial shear stress reaches its shear strength

$$\tau = \tau max \tag{8}$$

Then by substituting Eq. (8) into Eq.(5) a boundary condition for particle/matrix interfacial fracture can be established whereby,

$$\tau_{max} < \frac{n\sigma_p}{2} \tag{9}$$

This approach suggests that the outcome of a matrix crack impinging on an embedded particle depends on the balance between the particle strength and the shear strength of the interface.

A linear stress–strain relation [15-18] at the macro level can be formulated as follows:

$$\bar{\sigma} = \bar{C}\bar{\varepsilon} \tag{10}$$

where $\bar{\sigma}$ is macro stress, and $\bar{\varepsilon}$ represents macro total strain and $\bar{C}$ and is macro stiffness matrix.

For plane strain conditions, the macro stress- macro strain relation [13, 14] is as follows:

$$\begin{Bmatrix} \overline{\sigma_x} \\ \overline{\sigma_y} \\ \overline{\tau_{xy}} \end{Bmatrix} = \begin{bmatrix} \overline{C_{11}} & \overline{C_{12}} & 0 \\ \overline{C_{21}} & \overline{C_{22}} & 0 \\ 0 & 0 & \overline{C_{33}} \end{bmatrix} \times \begin{Bmatrix} \overline{\varepsilon_x} \\ \overline{\varepsilon_y} \\ \overline{\gamma_{xy}} \end{Bmatrix} \tag{11}$$

The interfacial tractions can be obtained by transforming the micro stresses at the interface as given in Eq. (3):

$$t = \begin{Bmatrix} t_z \\ t_n \\ t_t \end{Bmatrix} = T\sigma \tag{12}$$

$$\text{where, } T = \begin{bmatrix} 0 & 0 & 0 \\ \cos^2\theta & \sin^2\theta & 2\sin\theta\cos\theta \\ -\sin\theta\cos\theta & \sin\theta\cos\theta & \cos^2\theta - \sin^2\theta \end{bmatrix}$$

AA1100 alloy was used as the matrix material. The filler material was ZrC of average size 100nm. The material properties are given in table 1. The volume fractions of ZrC nanoparticles were 10% and 30%. A square RVE (Fig. 1) was modeled to compute the thermoelastic behavior AA1100 alloy/ZrC nanocomposites. The PLANE183 element was used to discretize the matrix and nanoparticle. The interphase between the nanoparticle and matrix was discretized with CONTACT172 element [21]. Both isothermal and hydrostatic pressure loads were applied at simultaneously on the RVE models.

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Table 1: Mechanical properties of AA1100 matrix and ZrC nanoparticles

Property	AA1100	ZrC
Density, g/cc	2.71	6.73
Elastic modulus, GPa	68.9	430
Ultimate tensile strength, MPa	110	874
Poisson's ratio	0.33	0.25
CTE, μm/m-^{o}C	21.8	6.8
Thermal Conductivity, W/m-K	220.0	25
Specific heat, J/kg-K	904	368
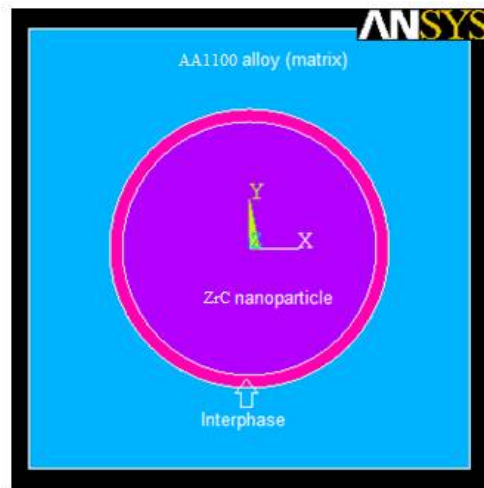
Fig.1. The RVE model.

III. **RESULTS AND DISCUSSION**

The influence of CTE on interface debonding and particulate fracture was assessed in terms of stress-strain relations, interfacial normal and tangential tractions and elastic modulus.
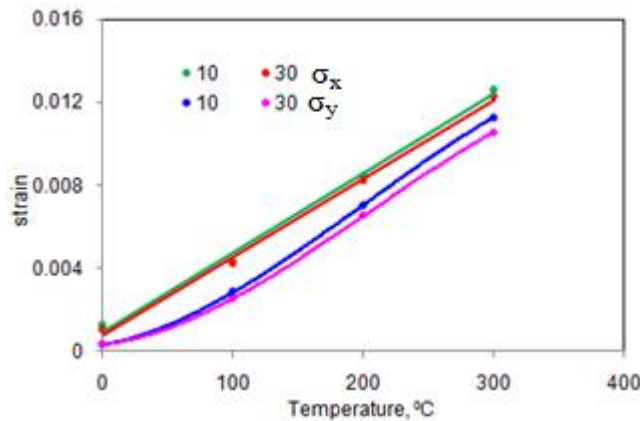

Fig. 2. Influence of temperature on thermoelastic strain.

A. *Micromechanics of thermo-elastic behaviour*

As the temperature increased, the strains become much larger than the experimental data because the softening occurs in the nanocomposites (Fig. 2). Due to high ductility and thermal expansion of AA1100 alloy matrix, the strains developed in it were higher than those of ZrC nanoparticles (Fig. 3).
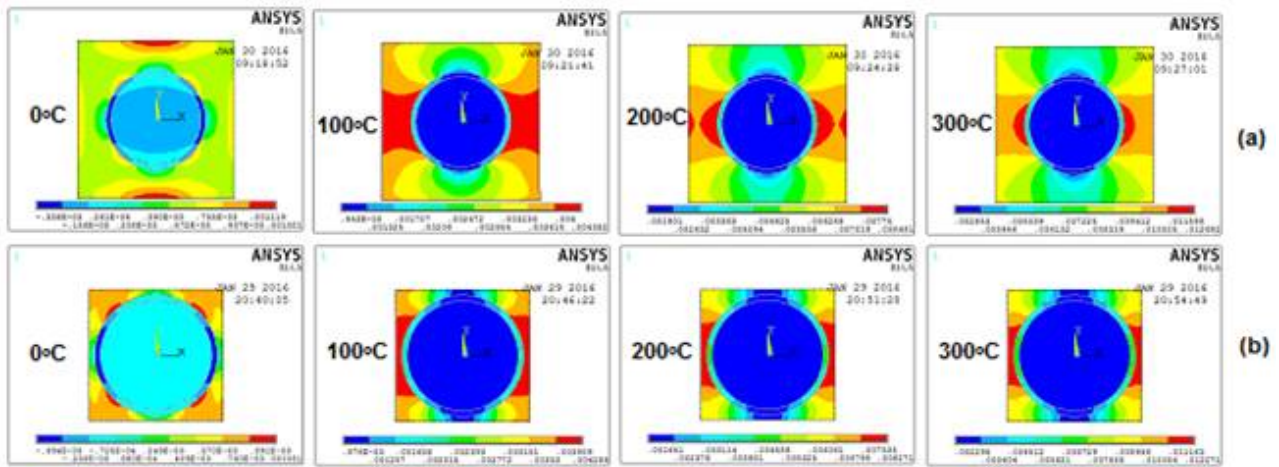

Fig.3. Raster images of tensile strains induced in (a) AA1100/10%ZrC and (b) AA1100/30% ZrC composites.

The stresses induced in the composites increased with the increase of temperature as shown in Fig. 4. The stresses are higher along the tensile load direction than those developed along the transverse direction of loading. This reveals a progressive shift from local plastic flow to bulk flow of matrix material because of temperature instigated softening.
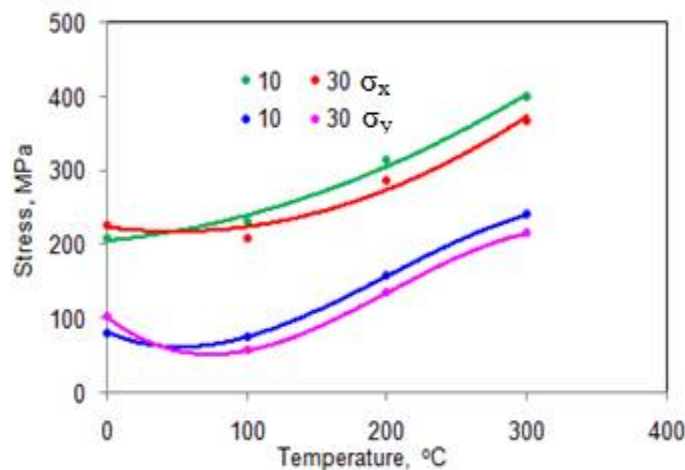

Fig. 4. Influence of temperature on strength.

Fig 5 shows tensile stresses obtained by the finite element analysis in the composites having 10% and 30% ZrC nanoparticles. The stress was very high either in ZrC nanoparticles or at the interphase on account of load transfer from the matrix to the nanoparticle. The elastic moduli (E_x and E_y) and major Poisons ratio (v_{12}) were evaluated for volume fractions from 10% and 30%. The tensile elastic modulus decreased with the increase of temperature (Fig. 6a). The major Poisson's ratio increased with increase of temperature (Fig. 6b).
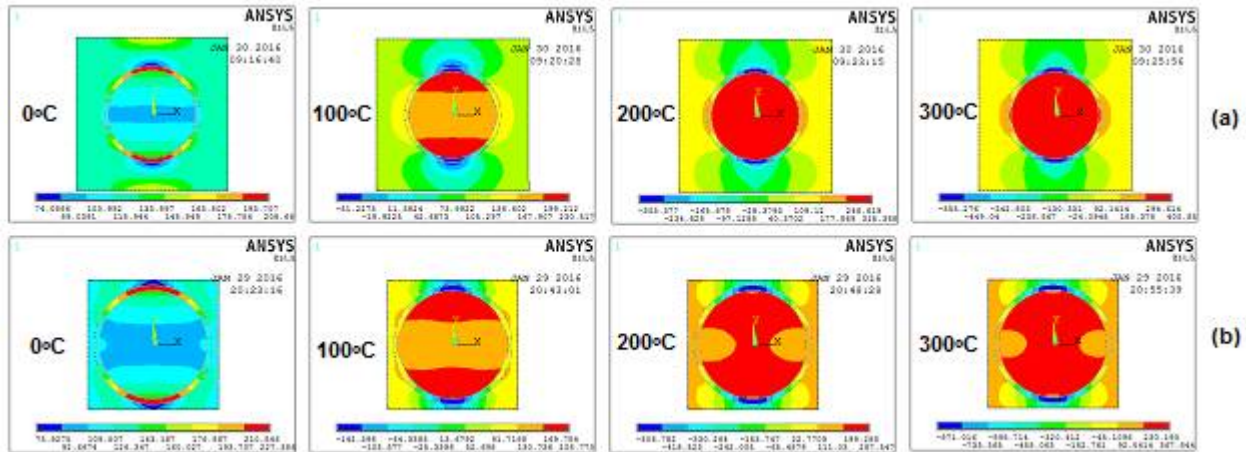
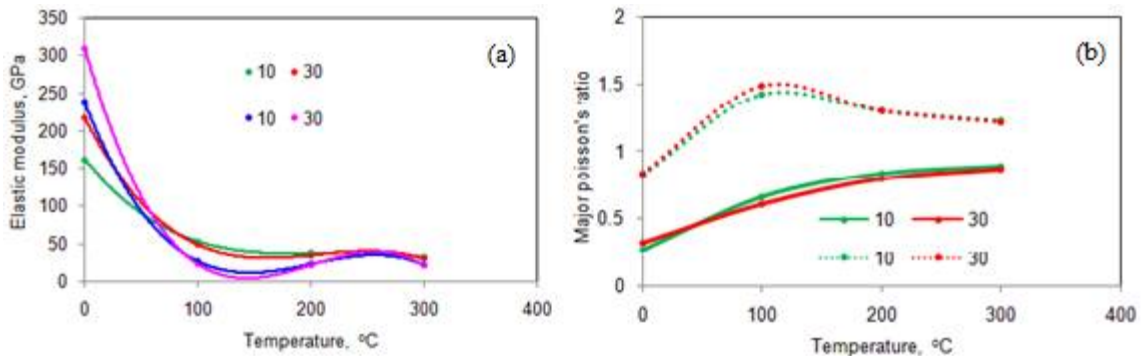Fig. 5. Raster images of tensile stresses induced in AA1100/10% ZrC and (b) AA1100/30% ZrC composites.

Fig. 5. Influence of temperature on (a) Ex, (b) Ey and (c) major Poisson's ratio.

B. *Debonding and particle fracture*

Influence of temperature on failure criteria in the composites is shown in Fig. 6. It is observed that the particulate fracture has occurred above $100^{o}C$ as the condition $\sigma_p < 2\tau/n$ is satisfied (Fig. 6a) for the composites having 10%ZrC particulates while it is above $75^{o}C$ for the composites comprising 30%ZrC particulates. The debonding of interface/interphase has occurred below $100^{o}C$ (Fig. 6b).
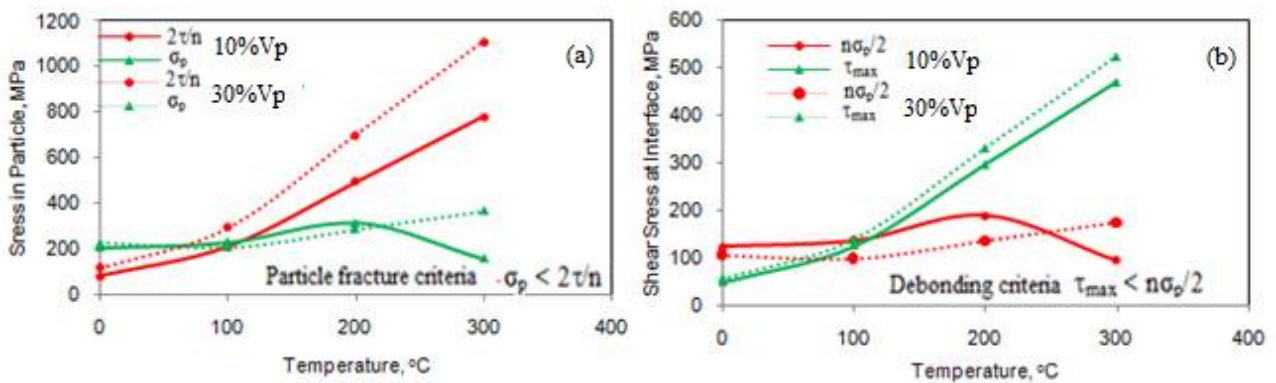

Fig. 6. Failure criteria: (a) Particulate fracture and (b) interface debonding.

The scanning electron microscope (SEM) image (Fig. 7) demonstrates the interface rupture in the composites having 30%ZrC at 100°C. Tear bands are also seen in the ZrC nanoparticulate due to CTE mismatch between the ZrC particulate and AA1100 alloy matrix.
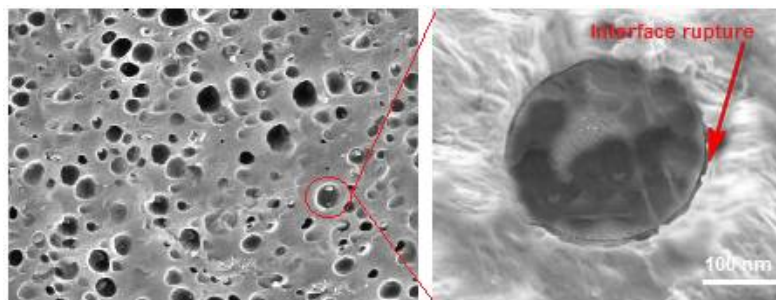

Fig. 7. SEM images illustrating rupture of interphase and tear bands in nanoparticles at 100°C.

IV. CONCLUSIONS

The fracture of ZrC nanoparticulate is highly dependent on the temperature. The debonding of interface has occurred below 100°C and ZrC particulate fracture has resulted above 100°C. The likelihood of particulate fracture was high in the composites having 30%Vp of ZrC. The stiffness of ZrC/AA1100 alloy metal matrix composites decreased with the increase of temperature.

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