Cohesive Zone Finite Element Analysis to Envisage Interface Debonding in AA7020/Titanium Oxide Nanoparticulate Metal Matrix Composites

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Abstract: A square array unit cell/2-D rectangular particulate RVE models were used to estimate interface debonding using cohesive zone analysis. The particulate metal matrix composites are titanium oxide/AA7020 alloy at different volume fractions of titanium nitride. Interface debonding was observed in all the composites. The interface debonding occurred between $0^\circ \leq \theta \leq 65^\circ$ in one-fourth model of symmetric geometry of AA7020/TiO$_2$ composites.

Keywords: AA7020, titanium oxide, rectangular particulate, RVE model, finite element analysis, interface debonding.

1. INTRODUCTION

Cell methods become widely used, which are based on the concept of a Representative Volume Element (RVE). The unit cell methods can easily account for complex microstructural morphology. Furthermore, finite element method is a most straightforward and common method for analyzing and modeling complex structures [1]. Multiphase finite element method is developed for modeling deformation and damage in particle-reinforced composite materials. Interfacial debonding is accommodated by cohesive zone models, in which normal and tangential spring tractions are expressed in terms of interfacial separation [2-15]. The criterion to an interfacial debonding is defined by the maximum normal tensile stress at the nodes of the matrix-inclusion interface. The cohesive zone is considered to be a fracture process zone ahead of the crack tip as illustrated in figure 1 for an infinite plate with a crack. Many different cohesive laws with variances in maximum traction, maximum separation, and shape have been proposed, such as the linear softening cohesive law by Camacho and Ortiz [16], the exponential cohesive law by Needleman [17] and Xu and Needleman [18], the trapezoidal cohesive law by Tvergaard and Huchinson [19], and the polynomial cohesive law by Tvergaard [20].

2. MATERIALS AND METHODS

The volume fractions of titanium nitride used in the present work were 10%, 20%, and 30% TiO$_2$. The matrix material was AA7020 alloy. The periodic model for the representative volume element (RVE) scheme was constructed from 2-D rectangular particulates in a square array distribution.
nanoparticulate. The cohesive zone can be incorporated in the continuum formulation by applying the cohesive tractions as boundary conditions. When the discretization is set up, two types of elements are required. One element is a continuum type element and the other a CZM type element. The Newton-Raphson Method (NRM) is used as it supports the concept of a tangent stiffness matrix. The cohesive element is implemented as a linear element with four nodes. The isoparametric formulation is chosen for the element, meaning that shape and displacements are interpolated by the same shape functions. Introducing the natural coordinate system, the linear Lagrangian shape functions are given as:

\[
\begin{align*}
N_1 &= \frac{1}{4}(1 - \xi)(1 - \eta) \\
N_2 &= \frac{1}{4}(1 + \xi)(1 - \eta) \\
N_3 &= \frac{1}{4}(1 + \xi)(1 + \eta) \\
N_4 &= \frac{1}{4}(1 - \xi)(1 + \eta)
\end{align*}
\]

(1)

Figure 2: The RVE model: (a) particle distribution and (b) RVE scheme.

Introducing the shape function matrix as:

\[
[N] = \begin{bmatrix}
N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 & 0 & 0 \\
0 & N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 & 0 \\
0 & 0 & N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4
\end{bmatrix}
\]

(2)

The displacements as functions of the natural coordinates can be written in the matrix-vector form as:

\[
\begin{align*}
\{u^+\} &= [N]\{q^+\} \\
\{u^-\} &= [N]\{q^-\}
\end{align*}
\]

(3)

Shear-log model is based on the assumption that all of the load transfer from matrix to particulate occurs via shear stresses acting on the particulate interface between the two constituents. The rate of change of the stress in the particulate to the interfacial shear stress at that point and the particulate radius, ‘r’ is given by:

\[
\frac{d\sigma_p}{dx} = -\frac{2\tau_i}{r}
\]

which may be regarded as the basic shear lag relationship.

The stress distribution in the particulate is determined by relating shear strains in the matrix around the particulate to the macroscopic strain of the composite. Some mathematical manipulation leads to a solution for the distribution of stress at a distance ‘x’ from the mid-point of the particulate which involves hyperbolic trig functions:

\[
\sigma_p = E_p\varepsilon_c[1 - \cosh(nx/r)\text{sech}(ns)]
\]

(5)

where \(\varepsilon_c\) is the composite strain, \(s\) is the particulate aspect ratio (length/diameter) and \(n\) is a dimensionless constant given by:

\[
n = \left[\frac{2E_m}{E_p(1+\psi_m)n(1+\psi_p)}\right]^{1/2}
\]

(6)
in which \( v_m \) is the Poisson ratio of the matrix. The variation of interfacial shear stress along the particulate length is derived, according to Equation (4), by differentiating this equation, to give:

\[
\tau_i = \frac{ nx }{ 2 } E_p \sinh \left( \frac{ ns }{ \tau } \right) sech(ns)
\]  

(7)

The equation for the stress in the particulate, together with the assumption of a average tensile strain in the matrix equal to that imposed on the composite, can be used to evaluate the composite stiffness. This leads to:

\[
\sigma_c = \varepsilon_c \left[ \nu_p E_p \left(1 - \tanh(ns) \right) + (1 - \nu_p)E_m \right]
\]  

(8)

The expression in square brackets is the composite stiffness. The stiffness is a function of particulate aspect ratio, particulate/matrix stiffness ratio and particulate volume fraction.

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

\[
\tau = \frac{n}{2} \sigma_p
\]  

(9)

If particle fracture occurs when the stress in the particulate reaches its ultimate tensile strength, \( \sigma_{p,uts} \), then setting the boundary condition at

\[
\sigma_p = \sigma_{p,uts}
\]  

(10)

and substituting into Equation (9) gives a relationship between the strength of the particle and the interfacial shear stress such that if

\[
\sigma_{p,uts} < \frac{\tau_t}{n}
\]  

(11)

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

\[
\tau = \tau_{max}
\]  

(12)

For particle/matrix interfacial fracture can be established whereby,

\[
\tau_{max} < \frac{nx}{2} \sigma_p
\]  

(13)

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.

For plane strain conditions, the macro stress- macro strain relation is as follows:

\[
\begin{bmatrix}
\bar{\sigma}_x \\
\bar{\sigma}_y \\
\bar{\tau}_{xy}
\end{bmatrix} = \begin{bmatrix}
\bar{C}_{11} & \bar{C}_{12} & 0 \\
\bar{C}_{21} & \bar{C}_{22} & 0 \\
0 & 0 & \bar{C}_{33}
\end{bmatrix} \times \begin{bmatrix}
\bar{\varepsilon}_x \\
\bar{\varepsilon}_y \\
\bar{\gamma}_{xy}
\end{bmatrix}
\]

(14)

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

\[
t = \begin{bmatrix}
\bar{t}_x \\
\bar{t}_y \\
\bar{t}_{xy}
\end{bmatrix} = T \sigma
\]

(15)

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

Figure 3: Effect of volume fraction on effective material properties.
3. RESULTS AND DISCUSSION

The tensile modulus increased \((141.76 < 142.62 < 143.83 \text{ GPa})\) with volume fraction of titanium oxide \((\text{TiO}_2)\) as shown figure 3a. Compression modulus was, respectively, 91.46 GPa, 89.69 GPa and 98.62 of AA7020/10% TiO\(_2\), AA7020/20% TiO\(_2\) and AA7020/30% TiO\(_2\) composites; whereas shear modulus was, respectively, 32.34 GPa, 32.60 GPa and 31.56 of AA7020/10% TiO\(_2\), AA7020/20% TiO\(_2\) and AA7020/30% TiO\(_2\) composites. The major Poisson's ratio decreased with increase of volume fractions of TiO\(_2\) (figure 3b). The difference in the elastic moduli of TiO\(_2\) particulates and AA7020 alloy matrix is 216 GPa. The Poisson’s ratios of AA7020 alloy matrix and TiO\(_2\) particulates are, respectively, 0.33 and 0.29.

![Figure 4](image_url)

**Figure 4:** Fracture criteria of: (a) particulate fracture and (b) interface debonding.

The TiO\(_2\) particulate fracture was not exposed in the AA7020/TiO\(_2\) composites as shown in figure 4a. The TiO\(_2\) particulate fracture was not produced as the condition \(\sigma_p \leq 2\tau/n\) did not satisfied. The condition \(\tau_{\max} < n\sigma_p/2\) satisfied for the occurrence of debonding in the composites including 10%, 20% and 30% TiO\(_2\) (figure 4b). The strain energy density decreased at the interface with an increase in the volume fraction of TiO\(_2\). Also, the strain energy density of TiO\(_2\) decreased in the composites. This represents the debonding tendency at the interface between AA7020 alloy matrix and TiO\(_2\) nanoparticles. The decreased strain energy density attributes to the interface debonding. The strain energy density in the TiO\(_2\) nanoparticles was lower than that developed in the matrix and at the interface. The normal and tangential tractions are plotted in figure 6a. Because of symmetry considerations, the variations of the interface stresses with circumferential location are plotted only for the range \(0^\circ \leq \theta \leq 90^\circ\). For AA7020/30%TiO\(_2\) composites, the normal tractions are higher than that for AA7020/10%TiO\(_2\) and AA7020/20%TiO\(_2\) composites (figure 6a). These results can be interpreted that the particulates are far enough apart at 10% particulate fiber volume fraction. This means that they do not interact (i.e., any particular particulate does not feel the influence of the other particulates in the neighborhood). At 10% particulate fiber volume fraction of TiO\(_2\) the particulates are close...
enough together that any individual particulate feels the influence of neighboring particulates. The interface debonding occurred between $0^\circ \leq \theta \leq 65^\circ$. The normal and tangential displacements are also plotted in figure 6b. The normal and tangential displacements are higher for AA7020/30%TiO$_2$ composites than those for AA7020/10%TiO$_2$ and AA7020/20%TiO$_2$ composites.

As the raster images (figure 7) obtained from finite element analysis, the interface debonding is highest in AA7020/30%TiO$_2$ composites. The images (figure 8) obtained from the scanning electron microscopy confirm the results obtained from the finite element analysis. The areas representing ‘A’ are the debonding zones and “B” represents the tear bands TiO$_2$ particulates.
4. CONCLUSION
The interface debonding occurred in the composites containing 10%, 20% and 30% volume fractions TiO$_2$; Nanoparticulate damage had not occurred. The interface debonding increased with an increase of volume fractions of TiO$_2$ in the composites. The interface debonding occurred between $0^\circ \leq \theta \leq 65^\circ$ in one-fourth model of symmetric geometry of AA7020/TiO$_2$ composites.

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