

Finite element study of interfacial effects in the consolidation of matrix coated fibre composites

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Abstract

The paper addresses finite element studies of the diffusion bonding effects at the interface between a locally reinforcing metal matrix composite and a monolithic engineering material. Diffusion bonding occurs during the consolidation of the composite during component manufacturing. The surface interaction behaviour at the interface has been described using an interface model. The model is developed by adopting an existing diffusion bonding theory and has been implemented into finite element software, ABAQUS, by mean of a user subroutine. Simulations of the surface interaction behaviour between the contacting surfaces have been carried out. The finite element simulations show that the diffusion bonding can lead to localized deformation, the inhibition of consolidation, and a resulting inhomogeneous distribution of consolidated and unconsolidated material which results from the constraint imposed on the consolidating composite.

1. Introduction

Continuous ceramic fibre reinforced titanium alloys are being developed for aerospace applications. They are generally used as local reinforcement in otherwise monolithic material components. Such locally reinforced composite components can be produced by inserting a bundle of continuous fibres, which are pre-coated with the titanium alloy matrix, into recesses machined into components also made from the titanium alloy. The application of pressure at an appropriate temperature causes the consolidation of the composite and also allows the fibre coatings, which are in intimate contact with the sides of the recess, to diffusion bond to the component. The surfaces of the component material and the matrix coating are not entirely flat as shown schematically in figure 1. When they are brought into contact, micro-cavities can

result. As time proceeds, the asperities on the contacting surfaces are flattened and the micro-cavities reduce in size. When the surfaces are fully bonded (that is, all the micro-cavities are removed), the matrix coating on the bond plane will no longer be able to slide relative to the contacting surface. The interface is, therefore, in a state of 'sticking friction'. This phenomenon can lead to the constraint of the deformation of the matrix coating during consolidation which in turn can inhibit subsequent consolidation resulting in a non-uniform consolidation as shown, for example, in figure 2.

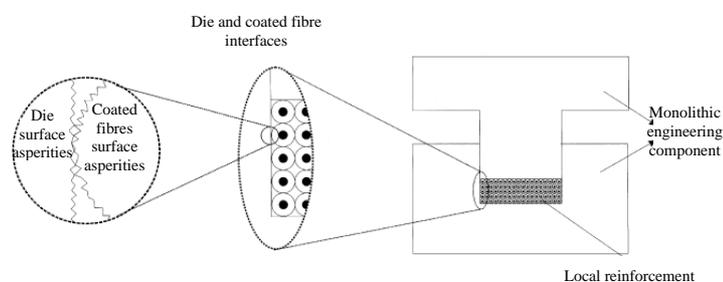


Figure 1 Schematic diagram showing the interface region between recess and coated fibres.

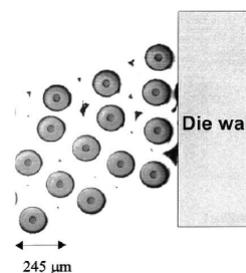


Figure 2 Micrograph showing a matrix-coated composite specimen consolidated after 1 h.

The effects of diffusion bonding at the interface between the bulk and composite materials are therefore significant and must be understood.

An interface model, which is able to describe the surface interaction behaviour at the interface between the bulk material and composite, has been developed which takes account of diffusion bonding. The interface model is then implemented into a finite element solver by mean of a user subroutine. The investigations of the diffusion bonding effects at the interface are carried out using a micromechanical finite element model. Simulation results are compared with experimental results

2. Development of interface model and its finite element implementation

An interface model has been developed to describe the interaction between the consolidating composite and the bulk material. The diffusion bonding process largely governs the frictional behaviour at the die-matrix coating interfaces. The interface model, therefore, takes account of diffusion bonding. By employing a diffusion bonding model, it becomes possible to determine when the surfaces are fully bonded and hence when a state of sticking friction takes place.

The bonding time can be calculated using Pilling's model [1]. The total rate of change of the cavity volume with time is given by

$$\left. \frac{dV}{dt} \right|_{total} = \left. \frac{dV}{dt} \right|_r + 2 \sum_0^{(N_j-1)/2} \left. \frac{dV}{dt} \right|_{r'} \quad (1)$$

This consists of mass transfer from the bond line and the sum of the mass transfers from each grain boundary intersecting the cavity. The first term is given by

$$\left. \frac{dV}{dt} \right|_r = \frac{16D_B \delta \Omega \sigma_c}{BA_f kT} \times \frac{1}{4 \ln \left(\frac{B+r}{r} \right) - \left[3 - \left(\frac{r}{r+B} \right)^2 \right] \left[1 - \left(\frac{r}{r+B} \right)^2 \right]} \quad (2)$$

where σ_c is the contact stress, D_B is the grain boundary diffusivity, Ω is the atomic volume, δ is the grain boundary width, r is the instantaneous radius and B is the diffusion distance defined as

$$B = \left| \frac{D_B \delta \Omega \sigma_c}{A_f kT \dot{\epsilon}} \right|^{\frac{1}{3}} \quad (3)$$

The second term, $\sum_0^{(N_j-1)/2} \left. \frac{dV}{dt} \right|_{r'}$, is the contribution to cavity

closure rate from the intersection between grain boundaries and the cavity surface. If the grain size is smaller than the interfacial cavity size, a number of paths exist by which diffusion can occur to sinter the cavity. The number of paths contributing to the closure of the cavity depends on the instantaneous radius (r) and the grain size (d) as the grain boundaries are assumed to lie parallel to the bond interface where the spacing between each layer is the same as the grain size. Thus, the number N_j of paths contributing to the closure of the cavity at any time is

$$N_j = 2 \text{int} \left(\frac{r}{d} \right) + 1 \quad (4)$$

The rate of change of cavity volume due to mass transfer from each grain boundary intersecting with the cavity can be determined from equations (3) and (4) by replacing instantaneous radius r and the area fraction bonded A_r by the apparent cavity radius r' and the apparent area fraction bonded A_f' in which

$$r' = \sqrt{r^2 - (jd)^2} \quad (5)$$

$$A_f' = 1 - \frac{r'}{r_0} \quad (6)$$

where r_0 is the initial cavity radius and j is an integer between 0 and $\left(\frac{N_j - 1}{2} \right)$.

Equation (1) has been derived for calculating a bonding time for a particular applied stress. In the present problem, the contact pressure between the coated fibres and the die walls varies during the consolidation. It generally decreases with time because the contact area between the coated fibres and the die walls increases with time. Additionally, not all of the surface of the matrix coating at the bond plane is fully bonded at the same time since the contact area progressively increases with deformation. Some parts on the bond plane may have already developed full interfacial contact but others may have just come into contact. In order to implement the diffusion bonding model, the area fraction bonded, A_r is employed to identify the state of full bonding, i.e. $A_r=1$. By rearranging equation (1), the increment in area fraction bonded (δA_r) for each time increment (δt) and for a given stress (σ_c) at that increment may be obtained

$$\delta A_f = \frac{\delta t}{-2\pi r_0^2} \left(\frac{dV/dt}{1-A_f} \right)_{total} \quad (7)$$

$\frac{dV}{dt_{total}}$ is given in equation (1). A_f is the area fraction bonded at the beginning of the time increment. A_f at the end of time increment can then be obtained by adding δA_f to the current A_f .

The finite element software, ABAQUS, provides a user subroutine FRIC to enable users to define alternative friction behaviour between contacting surfaces. Thus, the diffusion bonding model discussed here can be implemented into the finite element solver by means of this user subroutine. The increment in area fraction bonded, δA_p , is determined using information passed into the subroutine by ABAQUS, i.e. time increment (δt) and contact pressure (σ_c). The area fraction bonded, A_p , is assigned as a solution state variable and is updated every time increment. It is difficult to quantify at what value of A_f , relative sliding between the contacting surfaces ceases. However, it is certain that at the fully bonded state, (i.e. $A_f = 1$), the friction condition between the contacting surfaces becomes 'sticking'. In the initial development of the interface model, it is assumed that the friction condition is sticking when full interfacial contact is achieved. Otherwise, frictionless sliding is assumed. The value of A_f is used as a variable to specify when sticking friction occurs. If A_f is less than 0.99999 (A_f cannot be exactly equal to 1 for numerical reasons) then the friction condition is specified to be frictionless sliding. If A_f is greater than 0.99999 then the friction condition is specified to be sticking.

3. Micromechanical model for the interface problem

A finite element model has been developed to study the diffusion bonding effects at interfaces between die walls and coated fibres. Modelling a complete specimen is very much computationally prohibitive. Therefore, only a single column of coated fibres, which is in contact with a die wall, is considered. The interface area consists of a rigid die wall and five coated half fibres as shown in figure 3. The die is modelled using two-dimensional rigid elements (Left boundary) for which the reference nodes are not allowed to move or rotate. Fibres are assumed to be rigid and are defined as analytical surfaces in contact with the matrix. Perfect bonding is assumed for the fibre-matrix interfaces. Finite element meshes for the matrix material consist of four-noded, two-dimensional plane strain elements. Modelling contact problems in ABAQUS often leads to difficulties especially for contacts between two deformable bodies. Fine meshes are preferable for contact simulations but can give rise to computational cost. However, coarse meshes can lead to

unstable analyses. A few trial simulations have been carried out to obtain reasonable numbers of elements for the matrix-coated fibres, each of which contains 150 elements. The matrix is assumed to obey power-law creep behaviour. It has been found from the surface roughness measurement of a matrix-coated fibre that surface roughness of the matrix coating is very small, i.e. in the submicron range [2]. It is believed that the matrix coating surfaces will quickly diffusion bond to one another. Therefore, it is reasonable to assume sticking friction between the matrix-matrix interface. The diffusion bonding behaviour at the die-composite interface is described by the model detailed in the previous section.

An upper movable boundary is used for application of the distributed load, simulating the pressure state during the consolidation process. It is modelled using a two-dimensional rigid element. Its movement is restricted to be in the y direction. Frictionless conditions are applied to the interface between the upper movable boundary and the composite. All nodes on the right boundary including reference nodes of each fibre are only allowed to move in the y direction.

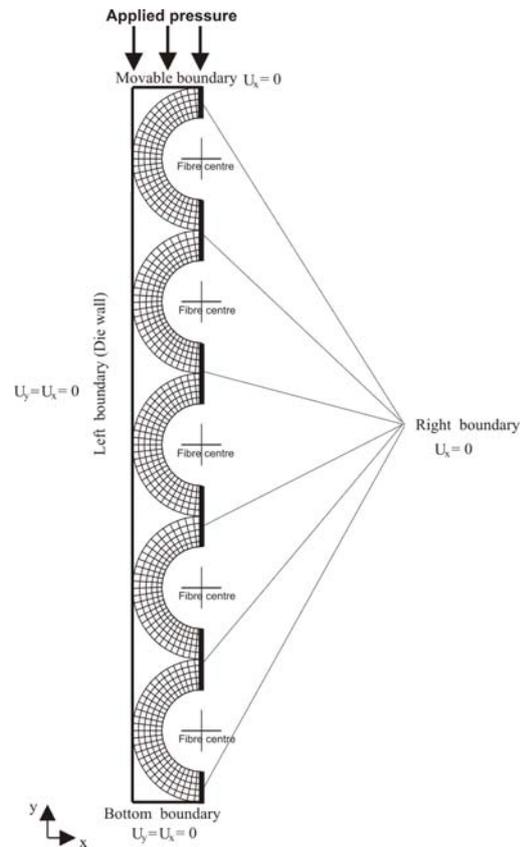


Figure 3 Schematics diagram showing the boundary and loading conditions imposed in the finite element micromechanical model.

4. Theoretical study of parameters which influence friction conditions

It is important to understand the sensitivity of the change in the area fraction bonded to surface roughness geometry, material property and material grain size values. In this section analyses have been carried out to study the effects of material diffusivity on the evolution of the area fraction bonded, A_f and hence diffusion bonding time. All simulations were carried out at a constant temperature of 900°C. A constant pressure of 20 MPa was imposed onto the upper movable boundary generating a macroscopically uniaxial stress state in the deforming material. The yield stress (σ_y) is assumed to be 54MPa [3]. Material properties for α Ti and β Ti at 900°C are given in table1. The properties of the alloy were obtained using the law of mixtures.

Table1 Material properties for α Ti and β Ti (after Pilling et al. [1])

Properties	α Ti	β Ti
Atomic volume (Ω), m ³	1.76×10^{-29}	1.81×10^{-29}
Grain boundary width (δ), m	5.9×10^{-10}	5.72×10^{-29}
Boundary diffusion coefficient (pre exponent), (D_{B0}), m ² s ⁻¹	6×10^{-5}	9×10^{-6}
Boundary diffusion activation energy, (Q_b), kJ mol ⁻¹	97	153
Lattice diffusion coefficient (pre exponent), (D_{v0}), m ² s ⁻¹	8.6×10^{-10}	1.9×10^{-7}
Lattice diffusion activation energy, (Q_v), kJ mol ⁻¹	150	153

4.1 Influence of grain boundary diffusivity (D_B) on the rate of diffusion bonding

Simulations have been carried out for various values of the grain boundary diffusivity (D_B). The initial cavity radius (r_0) and the grain size were set to be 1 μ m and 10 μ m respectively to be physically representative. Since grain size was set to be greater than the initial cavity radius, the only path contributing to the diffusion is from the bond line. Figures 4(a), (b) and (c) show profiles of the matrix-coated fibres at the interface after they have been consolidated for 300s. Figure 4(a) is obtained from the simulation with the grain boundary diffusivity, D_B , of $2.4 \times 10^{-11} \text{ m}^2 \text{ s}^{-1}$. The die and the matrix-coated fibre surfaces have not yet fully bonded to each other. The friction condition at the interface is still frictionless sliding as A_f is still less than 1, in particular, $A_f = 0.5508$. The array of coated fibres uniformly consolidates. The void sizes are approximately the same. Figure 4(b) is obtained from the simulation with the grain boundary diffusivity, D_B , of $1.4 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$. Some parts of the interface areas have become fully bonded after consolidation for

109s. At these locations, therefore, a state of sticking friction occurs. The matrix coating of the top coated fibre which has fully diffusion bonded to the die has, as a result, been prevented from moving downward. The upper voids are smaller in area than the lower ones, i.e. $V5b < V4b < V3b$, due to the fact that the movement of the matrix at the interface is constrained by the sticking friction state. This results in localised consolidation. The results for the grain boundary diffusivity, D_B , of $6 \times 10^{-8} \text{ m}^2 \text{ s}^{-1}$ are shown in figure 4(c). In this case the interface area diffusion bonds more quickly, i.e. within 20s. Thus, the sticking friction state has been imposed more quickly. This leads to earlier localised consolidation. The coated fibres at the bottom of the fibre array in figure 4(c) consolidate less than those shown in figure 4(b) whereas the region of the top coated fibre in figure 4(c) consolidates more. In addition, the height of the fibre array in figure 4(b) is less than that of figure 4(c) since its downward movement has been inhibited earlier.

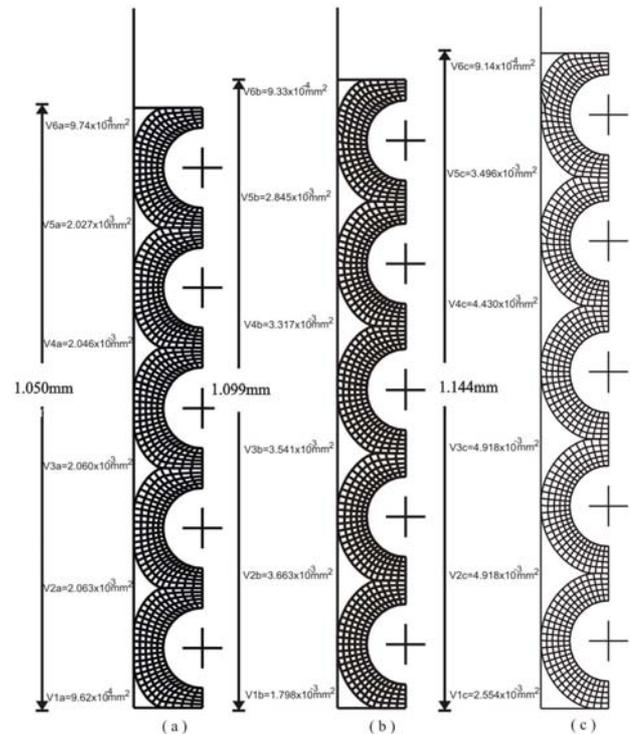


Figure 4 Computed finite element profiles after consolidation (a) $D_B = 2.4 \times 10^{-11} \text{ m}^2 \text{ s}^{-1}$ (b) $D_B = 1.4 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$ (c) $D_B = 6 \times 10^{-8} \text{ m}^2 \text{ s}^{-1}$

An early state of sticking friction is not desired in the processing of a reinforced composite component, as it leads to non-uniform consolidation and component distortion. An early state of sticking friction can be avoided by reducing the rate of diffusion bonding. The grain boundary diffusivity, D_B , is a temperature dependent material property normally given by

$$D_B = D_{B_0} e^{\frac{-Q}{RT}} \quad (8)$$

which increases with temperature. A lower consolidation process temperature therefore reduces grain boundary diffusion and hence inhibits the onset of sticking friction.

4.2 Influence of initial surface roughness on rate of diffusion bonding

Comparisons of the bonded area fraction (A_f) evolution over time for initial cavity radii of 1, and 5 μm have been obtained from the simulations with a grain boundary diffusivity D_B , of $1.4 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$ and grain size of $10 \mu\text{m}$. Figures 5(a) and (b) show profiles of the matrix-coated fibres at the interface for initial radii of 1 and 5 μm respectively after consolidation for 1400s. The simulation with a larger initial cavity radius shows a uniform consolidation. On the other hand, the simulation with a smaller initial cavity radius shows highly non-uniform consolidation. In conclusion, the surface preparation of the parts to be bonded is particularly important. Large initial cavity radius (r_0) leads to a slow diffusion bonding at the interface. Small initial surface roughness causes the die wall and the coated fibres to attain full interfacial contact more quickly which can result in unconsolidated dead zones.

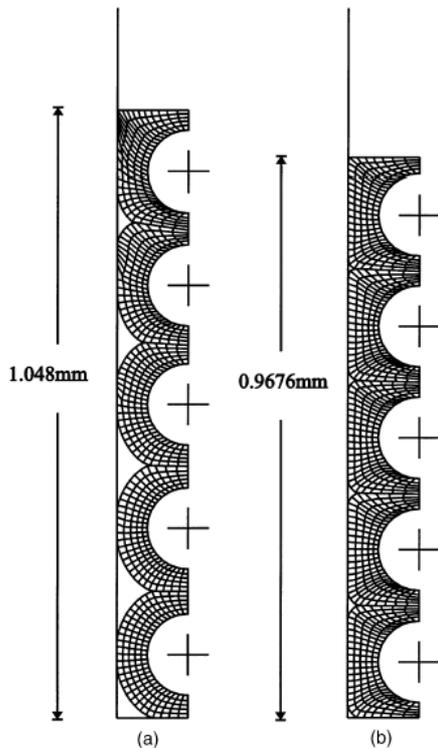


Figure 5 Computed finite element profiles after consolidation with (a) $r_0=1 \mu\text{m}$ (b) $r_0=5 \mu\text{m}$

5. Comparison of the model predictions with experimental results

Consolidation experiments have been conducted by Baik [2] to establish the validity of the model. In these experiments, a Ti-6Al-4V channel die without lubricant was used, into which was inserted unconsolidated composite material. In this way, the diffusion bonding behaviour between the Ti-6Al-4V die and the coated fibres could be investigated. The matrix-coated fibres were aligned and inserted into a Ti-6Al-4V channel die to form a composite specimen with square array packing. The radius of the coated fibre is 0.1225mm while the radius of the fibre only is 0.0705mm, i.e. the volume fraction of fibres is about 33%. The punch material used in this experiment was a nickel-based superalloy. The punch surface was lubricated. The specimens were then consolidated by uniaxial, vacuum hot pressing under a constant pressure of 20 MPa and at a constant temperature of 900°C . The test was interrupted after 300s. The specimen was sectioned after testing and the resulting microstructure is shown in figure 6(a). The micrograph shows that sticking friction has already occurred since the void sizes at the die-composite interface are different. The top layer of the coated fibres has been deformed more than the lower ones.

The same finite element model described earlier was used to simulate the experiment. The surface roughness of the die is about 1 μm . The matrix grains are plate-like with 1 μm width and 10 μm length. The grain size is, therefore, just larger than the cavity radius. Thus, it is assumed that it has no effect on the diffusion bonding. Two values of grain boundary diffusivity (D_B), $1.4 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$ (taken from [1] for αTi and βTi at 900°C) and $6 \times 10^{-8} \text{ m}^2 \text{ s}^{-1}$, were used. Figure 6(a) and 6(b) shows comparisons of the predicted profiles with the experimental micrographs for the grain boundary diffusivity of $1.4 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$ and $6 \times 10^{-8} \text{ m}^2 \text{ s}^{-1}$ respectively. Figure 6(a) shows that the void areas predicted by the model are comparable with the experimental results but the predicted height of the specimen is smaller than that of the experiment. A better comparison can be seen when using the grain boundary diffusivity of $6 \times 10^{-8} \text{ m}^2 \text{ s}^{-1}$ as shown in figure 6(b). However, the predicted height of the specimen is still slightly smaller than that of the experiment. The difference between the measured and the predicted height results from the sticking friction state which may actually take place before full diffusion bonding occurs at every point on the bond plane ($A_f=1$). When the level of the area fraction bonded, A_f , at which the friction condition becomes sticking was changed from 0.99999 to a smaller value, better agreement could be obtained.

However, it has not yet been possible to quantify the level of the area fraction bonded, A_b , at which the friction condition becomes 'sticking'. It should also be noted that friction effects before diffusion bonding occurs are ignored in the model. Further experimental investigations are required to give insight into the frictional behaviour of the materials at the interface prior to diffusion bonding. It is also useful to note that the grain boundary diffusivity is dependent on the proportion of β and α phase [1] at a particular temperature. The composition of each phase changes with temperature. The diffusivity data for Ti-6Al-4V taken from Pilling et al. [1] were calculated from those of the constituent phases by the law of mixtures. The volume fraction of β was assumed to be that given by experimentally determined temperature-volume fraction data for the β -phase. As a result the grain boundary diffusivity for PVD Ti-6Al-4V may be quite different from that of conventional Ti-6Al-4V. Indeed, microstructural examination shows that PVD Ti-6Al-4V has a much finer grain size and exhibits much higher creep rates than the conventional Ti-6Al-4V [4]. A larger diffusivity ($6 \times 10^{-8} \text{ m}^2 \text{ s}^{-1}$) for this material may well, therefore, be justified.

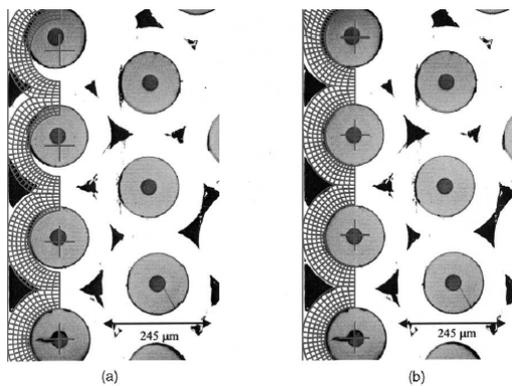


Figure 6 Comparison of predicted and experimentally observed consolidation of coated fibres in contact with a Ti-6Al-4V die (on the left). D_B of (a) $1.4 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$ and (b) $6 \times 10^{-8} \text{ m}^2 \text{ s}^{-1}$ were used.

6. Conclusions

A simple interface model was developed by adopting an existing diffusion bonding model to describe the surface interaction behaviour at the interface between bulk matrix material and matrix-coated fibre composites. By consideration of the area fraction bonded between the two contacting surfaces, friction conditions were specified. A micromechanical finite element model of a single column of coated fibres which was located at the interface was developed. The interaction behaviour between the contacting surfaces was described using the interface model. It was found that the grain boundary diffusivity and initial surface

roughness affect the diffusion bonding, and hence the friction condition at the interface. The higher the grain boundary diffusivity, the higher the rate of change in area fraction bonded, hence the earlier sticking friction between the contacting surfaces was achieved. Large initial surface roughness leads to a longer time to achieve full bonding. Thus, the state of sticking friction is delayed. Diffusion bonding between local reinforcing composite and monolithic matrix has been shown to lead to inhomogeneous consolidation.

The finite element predictions were also compared with experimental results. With the grain boundary diffusivity taken from [1], the void areas predicted by the model are in reasonable agreement with the experimental results but the predicted height of the specimen is shorter than that found in the experiments. The difference is possibly due to the fact that the state of sticking friction occurs before the contacting surfaces attain 100% bonding. However, it has not yet been quantified at which level of area fraction bonded is required for relative sliding between the contacting surfaces to cease. Better comparisons can be obtained using higher values of the grain boundary diffusivity.

7. Acknowledgement

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