SIMULATION OF MICROSTRUCTURAL EVOLUTION DURING TMC MONOTAPE CONSOLIDATION PROCESSING

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Abstract—The consolidation of fiber-reinforced titanium matrix composite (TMC) monotapec produced by spray deposition is an important step in the manufacture of TMC components. The performance of this class of composites is controlled by fiber-matrix properties and by the composite's relative density, fiber microbending stress/fracture and by the interfacial reaction layer thickness at the fiber-matrix interface after processing. These three microstructural features evolve during consolidation processing. Models for predicting the microstructure's dependence upon process conditions (i.e. the time varying pressure and temperature) are combined with consolidation equipment dynamics to simulate the microstructural evolution and to assess the relative "processibility" of several silicon carbide fiber-titanium alloy matrix systems during their transient consolidation processing. The dependence of the microstructural state upon the material system's mechanical properties and the monotape's initial geometry has also been investigated and is used to propose guidelines for the selection of TMC system materials and monotape geometry parameters.

1. INTRODUCTION

Continuous fiber-reinforced titanium matrix composites (TMCs) are being developed for a variety of applications in gas turbine engines and other aerospace structures [1, 2]. A critical enabling step in their development is the maturing of reliable low-cost processing methods capable of producing affordable high quality composites. In TMCs, aggressive chemical reactions between the high strength silicon carbide or aluminum oxide reinforcing fibers and the liquid matrix alloy precludes the use of low cost solidification processing pathways such as squeeze casting or pressure infiltration for the manufacture of composite components [3–6]. Approaches such as molten droplet spray deposition [7, 8], vapor phase deposition [9–11] and powder slurry (tape) casting [12] are instead under development. Each of these synthesis methods either minimizes or eliminates liquid matrix alloy-fiber contact during processing and results in the formation of a unidirectional fiber-reinforced sheetlike preform containing a single layer of roughly equi-spaced fibers in a sometimes porous alloy matrix [7]. A high temperature consolidation step is then used to produce a near net shape component from a layup of any of the preforms [13, 14].

The performance of the composites manufactured by this two step process sequence has sometimes been unsatisfactory and considerable experimental effort continues to be devoted to finding a successful process methodology [15, 16]. The reasons for this are now beginning to emerge: micromechanical modeling of composite performance attributes such as strength [17–19], crack growth resistance [18–20], creep rupture life [21, 22] and fatigue endurance [23] have all revealed the existence of a strong dependence of composite performance upon the fiber strength, the fiber-matrix sliding resistance, the matrix strength and the level of residual stresses formed during the consolidation process. The performance attributes are affected by the way in which processing is conducted. For example, longitudinal strength and crack growth resistance decrease when process conditions are used that cause either the sliding stress of the fiber-matrix interface to increase [24] or the fiber strength to be reduced (e.g. after prolonged high temperature consolidation cycles [25]). Fiber microbending stresses and fracture occur when differential densification rates exist along the fibers during processing [17], and this also leads to a loss of longitudinal composite strength [17], especially under creep conditions. Incomplete densification results in residual matrix porosity, which is likely to result in a loss of matrix strength and reduced transverse mechanical performance. Residual stresses due to coefficient of thermal expansion (CTE) mismatch between fibers-matrix-consolidation tooling increase with the consolidation temperature. They frequently leave the matrix in tension which can cause radial matrix cracking and additional loss in transverse properties [26].

For each of the monotapeces, the significance of these processing related effects upon the composite's performance is a function of the initial monotape
geometry (i.e. its surface roughness and internal porosity), various mechanical properties of the fiber–coating–matrix system and the precise temporal variation of the load and temperature applied during consolidation. Since so many factors affect the composite’s ultimate performance, and because the significance of each depends sensitively (and often non-linearly) upon the process conditions, the design of experiments methodology that might normally be used for refining a manufacturing process, in this case has proven to be time consuming, costly and in many cases appears to have arrived at sub-optimal solutions.

In an attempt to realize the full potential of these promising materials systems, several groups have sought to apply modeling approaches to improve process design [14, 27–42]. The micromechanisms responsible for densification, fiber microbending fracture, interfacial reactions, etc. have begun to be identified and predictive relationships developed linking them to the initial preform geometry, fiber–matrix properties and the pressure, temperature and time used for consolidation. In almost all cases, the process conditions have been implicitly held constant for the calculations, and the results have often been presented in the form of maps relating a microstructural parameter of interest to a pair of process variables (e.g. relative density to pressure and temperature) [14, 33]. These studies have revealed the need for careful trade-offs between pressure and temperature. For instance, highest relative densities are achieved by maximizing both the pressure and temperature. However, fiber microbending/fracture has been shown to be severe at high pressure unless low pressurization rates (i.e. long consolidation times) and high temperatures are used [43]. Unfortunately, these conditions promote both extensive interfacial reactions and large CTE difference derived residual stresses in the consolidated component [44]. Since the degree to which each of these effects occurs depends on properties of the TMC system components and the geometry of the monotape, the optimum trade-off will vary for different material systems, and a different process is likely to be required for each.

The modeling approaches reported to date have utilized hypothetical, overly simplistic process cycles: pressure and temperature are often implicitly assumed to be both instantaneously applied and in phase; they are normally maintained constant throughout the cycle, etc. In reality, the equipment used for consolidation has limited temperature and pressure capacities and finite heating/cooling and pressurizing rates. Furthermore, the temperature and pressure do not have to be ramped simultaneously (i.e. in phase), nor do they have to be maintained as constant throughout a consolidation cycle. In fact, dynamic adjustment to the conditions during a transient consolidation process might enable temporally varying trade-offs between temperature and pressure to be made in order to obtain fiber microbending, interfacial reaction thickness and relative densities that result in composites of better performance. These opportunities/constraints need to be included in the modeling approach if it is to be fully exploited for the design of composite manufacturing processes that in turn realize the maximum potential of this new materials class.

Given the complexity of the phenomena activated during titanium matrix composite consolidation, their sometimes significant interdependence, and the many (often poorly known) material and monotape geometry parameters needed as model inputs, it is unrealistic to expect that a modeling approach will exactly reproduce experiments. However, provided the models properly predict the important trends and give reasonable quantitative agreements (perhaps after the tuning of poorly known parameters using a few carefully controlled experiments) these models promise to significantly aid the development of acceptable processes and the selection of materials.

The study reported here reviews new results from contact and porous body micromechanics and uses them to revise models for the densification, fiber microbending and fiber–matrix reaction that accompany the consolidation of TMCs. It subsequently combines each of these microstructural evolution models with consolidation machine constrained, temporally varying pressure and temperature waveforms to simulate, the coupled simultaneous evolution of the microstructural states during the consolidation of plasma sprayed Ti–6Al–4V/SCS–6 TMC monotapes. The resulting dynamic model is used to assess the feasibility of successfully processing several other TMC systems of current interest. The simulation approach is shown to allow a rapid assessment of any composite systems “processibility” provided basic mechanical property/diffusion data are available for the material system. It also enables rapid trial and error testing for the design of a near optimal consolidation process cycle, and also facilitates identification of strategies for adjusting the spray deposition process to improve the processibility of more (difficult to process) deformation resistant matrix–small diameter fiber systems. Subsequent work combines the dynamic simulation methodology developed here with micromechanical structure–property models to obtain processing–performance relationships [45], with Monte-Carlo techniques to investigate the relations between process yield, quality and cost [46], and with optimization algorithms to design and control optimal consolidation process paths that lead to desirable “goal state” combinations of microstructures and properties at process completion [47, 48].

2. DYNAMIC MATERIAL MODELS

The consolidation of a spray-deposited TMC monotape layup is shown schematically in Fig. 1. Prior to consolidation, a layup typically contains
35-45% internal porosity, most of which forms between the monotapes as a consequence of their surface roughness. The remaining porosity exists as isolated internal voids created between solidified droplets during the spraying process. Upon application of an externally applied pressure, the laminate densifies by the inelastic contact deformation of surface asperities and by matrix flow around the isolated voids. The asperity's resistance to this inelastic flow leads to large localized contact stresses which cause fiber microbending and sometimes fiber fracture. The extended high temperature exposure of many commonly used consolidation cycles also results in temperature-dependent reactions between the fiber's coating and the matrix. Models relating layup relative density, fiber microbending/fracture and interfacial reaction product growth to the process conditions can be assembled from recent developments in contact mechanics [34, 35, 141, from new analyses of void collapse in power law creeping solids [49, 50], from calculations of fiber microbending/fracture [33] and from empirical kinetic models for fiber-matrix interfacial reactions [44]. The sometimes important coupling between densification and fiber microbending or between fiber fracture and interfacial degradation can also be included in the simulation by simultaneously (numerically) integrating the models and tracking the evolution of these “microstructural” states for any pressure-temperature history.

2.1. Densification

The prediction of the relative density of a spray-deposited TMC layup as a function of the applied stress, temperature and time has been greatly simplified by modeling each individual monotape as two sub-laminae: one, referred to as the “r”-lamina (reinforced), contains the array of fibers, has smooth sides and (up to 10%) internal porosity in the form of isolated voids while the other, the “s”-lamina (surface), consists of only the surface asperities (see Fig. 1).

Densification of the s-lamina has been analyzed in two sequential stages: “Stage I” densification occurs at lower relative densities $D_0 \leq D < 0.85$ (where $D_0$ is the initial relative density of the s-lamina) by the blunting of asperity contacts. At higher relative densities ($0.92 < D < 1$), referred to as “Stage II”, isolated voids have formed within the spaces between former asperities and densification is then more accurately described as the shrinkage of internal pores. The analysis of densification during both Stages I and II relies on a micromechanics approach in which the constitutive behavior of a representative volume of material is modeled and then used with a stochastic geometry model to predict the overall (macroscopic)
response. During Stage I, contact mechanics solutions are used to predict the relationship between forces arising at a contact as a result of externally applied loads and the resulting macroscopic deformation. The analysis of void shrinkage in Stage II has been treated by the application of variational principles of continuum mechanics to a single spherical void in an infinite matrix. An interpolation function has been used to approximate the transition behavior between Stages I and II for the s-layer in the regime $0.85 \leq D^v \leq 0.92$ [47]. Since the r-lamina has an initial relative density of about 0.9 or greater, and the porosity exists in the form of closed voids, it can be analyzed as just a Stage II problem, i.e. using results for void collapse that occur simultaneously with the s-lamina's densification.

Consolidation typically occurs over a wide range of temperatures, $0.2 \leq T/T_m \leq 0.8$, where $T_m$ is the absolute melting temperature, and applied pressures, $0 < P/\sigma \leq 0.8$, where $\sigma$ is the uniaxial yield strength. Thus, depending on the consolidation conditions, several deformation mechanisms could contribute to the overall densification rate at any time. The modeling approach does not rely on identification of a dominant deformation mechanism under a given set of processing conditions. Instead, the unit cell models for Stages I and II have been developed for time-independent plastic yielding, for power-law creep and for diffusional creep, respectively, and $s_l$, $s_d$ are the densification rates due to power-law relative density due to plastic yielding, $s_l$, $s_d$ and $s_r$ represent the contributions to $I$:

$$D'(t) = D_0 + \Delta D_p(t) + \int_0^t \left( \sum_{i=1}^2 s_i(D'_i(t) + D''_i(t)) \right) dt$$

(1)

$$D''(t) = D'_0 + \Delta D_p(t) + \int_0^t (D'_2(t)) dt.$$  

(2)

Here, $D'_0$ and $D'_2$ are the initial relative densities of the s- and r-laminae, $\Delta D'_p$ and $\Delta D''_p$ are the changes in relative density due to plastic yielding, $D'_1$, $D'_2$ and $D''_2$ are the densification rates due to power-law and diffusional creep, respectively, and $s_i$ represent smoothing functions used to interpolate between Stages I and II.

The temperature and stress dependence of the material parameters in these models together with the evolving system's geometry govern the relative importance of each mechanism. Equations (1) and (2) are solved by numerical integration over time, $t$, for a prescribed consolidation cycle defined by pressure, $P(t)$, and temperature, $T(t)$, waveforms. The composite's overall relative density ($D$) is given by

$$D(t) = D'(t)\nu'(t) + D''(t)\nu'(t)$$

(3)

where $\nu'(t)$ and $\nu'(t)$ are the volume fractions of the s- and r-layers, which change with time because the relative rates at which the s- and r-laminae densify are, in general, different.

A thin laminate made up of spray-deposited TMC monotapes subjected to a uniform pressure will experience densifying strains which are much greater in the through-the-thickness direction than in the plane of the laminate. The reasons for this are discussed in Ref. [14], however, the essential argument is that the high density and reinforcement of the r-laminae shields the very porous s-layers from in-plane loads. The densification model has thus been developed for the case of constrained uniaxial compression in which deformations only occur perpendicular to the plane of the laminate.

Stage I densification of the s-lamina is modeled as an assemblage of hemispherical asperities of statistically varying radius and height subjected to constrained uniaxial compression. While the original model used classical results from indentation theory to analyze the blunting of a single asperity contact (of arbitrary size), recent developments in contact mechanics have led to improved contact stress–blunting displacement relationships. In particular, the earlier model used, as the criterion for contact flow, the classical slip-line solution for a flat punch indenting a rigid, perfectly plastic half-space [14] by time-independent plasticity. A dimensional analysis was used to estimate the contact mechanics relationships for the case of steady-state creep. These have proven to be over simplified. Recent finite element analyses (FEA) of the elastic–plastic and elastic–power law creep blunting of contacts have led to more rigorous relationships between contact stress and blunting strain (rate) [34, 35].

FEA has identified two main contributions to an asperity's resistance to contact deformation. One arises from the elastically deformed material (or more slowly deforming material during creep) surrounding the zone of plastic deformation at the contact (material constraint). The other originates from the presence of neighboring asperities which impose a lateral constraint on blunting. For plasticity, the material constraint contribution to asperity blunting has been shown to depend on both the geometry (i.e. the shape) of the asperity (which changes with further blunting) and upon the matrix material's work-hardening rate.

If the criterion for plastic flow at a contact is written in the form

$$\sigma_c = Fe_\sigma,$$

(4)

where $\sigma_c = $ contact pressure and $\sigma$ is the matrix material's uniaxial yield stress, then $F$ is a flow (constraint) coefficient ($= 2.97$ for rigid–perfectly plastic indentation). Approximate analytical expressions have been developed for the evolving shape ($F_i$) and work hardening ($F_h$) contributions to $F$. 
in the presence of a density dependent lateral constraint

\[ F_r(D) = 34.44 D^2 - 58.04 D + 26.31 \]  

(5)

\[ F_u(D) = \frac{k}{r} \left[ \ln \left( \frac{0.202}{D^2} - \frac{0.703}{D} + 1.601 \right) \right]^r \]  

(6)

where \( k \) is the strain hardening coefficient, \( D \) is the relative density of the representative cell containing a single asperity (see Fig. 1) and \( p \) is the matrix material's work-hardening exponent. Gampala et al. [34] showed that to a good approximation, the blunting response for any work-hardening material can be obtained by summing these two contributions to the constraints.

Power law creep blunting of hemispherical asperities has been analyzed using a similar approach [35] and analogous approximate analytical expressions obtained for the contact flow stress and contact area evolution in terms of two non-dimensional coefficients \( F \) and \( C \)

\[ \frac{\sigma_c}{\sigma_o} = F(D, n) \left( \frac{h}{\ell_o a} \right)^n \]  

(7)

\[ h = \frac{1}{2(C(n))^2} \left( \frac{\sigma^2}{r} \right) \]  

(8)

where \( \sigma_o \) and \( \ell_o \) are reference stress and strain rates, \( n \) is the creep exponent in Norton's power-law for steady-state creep, \( a \) is the contact radius and \( r \) is the asperity's initial radius. \( C(n) \) relates the contact radius \( (a) \) to the blunting displacement \( (h) \), while \( F(n, D) \) generalizes the flow coefficient to creep and relates the mean contact stress \( (\sigma) \) to the blunting velocity \( (h) \), i.e., it is the time-dependent deformation analog of \( F \) defined in equation (4) and converges to the perfect plasticity result \( n \rightarrow \infty \). The blunting deformation \( (h) \) in equations (7) and (8) is defined as the difference between the initial asperity height and the blunted asperity height when the relative density increases from \( D_s \) to \( D' \). Approximate, density-dependent expressions for \( F(n, D) \) and \( C(n) \) have again been calculated by means of FEA for a wide range of \( n \)-values (Table 1).

The single-asperity contact analyses result in expressions for the contact force-density relations for (time-independent) plastic yielding, steady-state (power-law) creep and diffusional flow. These have been collected and are summarized in Table 2.

The overall response of the s-lamina is obtained by combining the predicted behavior for a single asperity with a statistical model incorporating the variation in asperity radius \( (r) \) and initial height \( (h) \) [14]. This introduces two probability distribution functions (PDFs), \( \varphi_r \) and \( \varphi_h \), representing the probabilities of encountering surface asperities of a given radius and height, respectively. The applied pressure, \( \Sigma \), necessary to achieve a prescribed densification rate will then be given by the sum of the forces acting on all the asperities per unit area.

If \( \gamma \) is the number of asperities per unit area, imposition of a force balance results in the desired Stage I macroscopic stress–density relation

\[ \Sigma(D', \delta') = \gamma \int_0^\infty \varphi_r(h) \varphi_h(r) \times F_k(h, r, D', \delta') \, dh \, dr, \]  

(9)

where \( z_0 \) is the initial s-lamina thickness and \( z \) corresponds to the thickness (or height) when the relative density has a value \( D' \). Equation (9) can be implicitly solved for the relative density provided the two probability distributions and the various material parameters identified in Table 2 are known. Examples of these parameters for two illustrative titanium alloys are given in Table 3.

### Table 1. Coefficients \( C(n) \) and \( F(n, D) \) for large displacement blunting [35]

<table>
<thead>
<tr>
<th>( n )</th>
<th>( C(n) )</th>
<th>( F(n, D) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.867</td>
<td>43.16 ( D^2 ) - 58.99 ( D ) + 21.12</td>
</tr>
<tr>
<td>2</td>
<td>0.923</td>
<td>39.67 ( D^2 ) - 60.29 ( D ) + 24.71</td>
</tr>
<tr>
<td>5</td>
<td>1.059</td>
<td>32.88 ( D^2 ) - 55.21 ( D ) + 25.01</td>
</tr>
<tr>
<td>10</td>
<td>1.112</td>
<td>36.77 ( D^2 ) - 60.55 ( D ) + 26.8</td>
</tr>
</tbody>
</table>

### Table 2. Expressions for unit cell model densification

<table>
<thead>
<tr>
<th>Deformation mechanism</th>
<th>Contact force-relative density relationships for Stage I densification</th>
<th>Deformation potentials for Stage II densification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plastic yielding [35, 14]</td>
<td>( F_z = 2\pi r \left( \frac{h - z_0 D_s}{D_s} \right) (F_z + F_r) )</td>
<td>( \phi \Sigma = \frac{\Sigma}{\sigma_0} + \left( -2\varphi (1 - D) \cosh \left( \frac{\Sigma z}{2\sigma_0} \right) \right) - 1 = 0 )</td>
</tr>
<tr>
<td>Power-law creep [36]</td>
<td>( F_z = \frac{\pi \sigma_o F(n, D)}{[2\pi h (\ln(\frac{D}{D_s}))^2 \ln(\frac{D}{D_s})]} )</td>
<td>( \phi = \frac{\pi}{n + 1} \left[ \sigma (D) \Sigma^2_{D_0} + h (D) \Sigma^2_{D_0} \right]^{1+1} )</td>
</tr>
<tr>
<td>Diffusional flow [14]</td>
<td>( F_z = \frac{c \sigma_o T}{12 \times (D_s + 2 \rho D_s)} \left( \frac{\sigma_0}{D_0} \right)^D )</td>
<td>( \phi = \frac{5 \text{ } \pi}{kT} \left( \frac{\delta D_0}{D_0} + \frac{2}{3} \rho D_0 \right) \Sigma^2_{D_0} )</td>
</tr>
</tbody>
</table>

\( k \) is Boltzman’s constant, \( T \) is the absolute temperature, \( \Omega \) is the atomic volume, \( \delta D_0 \) is the boundary diffusion mobility, \( \rho D_0 \) is the volume diffusion mobility, \( r \) is the radius of the hemisphere and \( g_r(D) \) is a polynomial function of the density.
Table 3. Matrix material parameters used for simulation studies [14]

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Symbol (units)</th>
<th>Ti-24Al-11Nb</th>
<th>Ti-6Al-4V</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting temperature</td>
<td>( T_m ) (K)</td>
<td>1875</td>
<td>1941</td>
</tr>
<tr>
<td>Atomic volume</td>
<td>( \Omega ) (m(^3)/atom)</td>
<td>( 1.0 \times 10^{-27} )</td>
<td>( 1.78 \times 10^{-27} )</td>
</tr>
<tr>
<td>Yield stress-temperature relation</td>
<td>( \sigma_y ) (MPa)</td>
<td>539.9-0.32T</td>
<td>884.0-0.92T</td>
</tr>
<tr>
<td>Young's modulus-temperature relation</td>
<td>( E ) (GPa)</td>
<td>1019.9-0.92T</td>
<td>115-0.056T</td>
</tr>
<tr>
<td>Power-law creep constant</td>
<td>( A ) (l/h)</td>
<td>6 \times 10^{-17}</td>
<td>8.4 \times 10^{24}</td>
</tr>
<tr>
<td>Power-law creep exponent</td>
<td>( n )</td>
<td>2.5</td>
<td>4.0</td>
</tr>
<tr>
<td>Power-law creep activation energy</td>
<td>( Q_c ) (kJ/mol)</td>
<td>285</td>
<td>280</td>
</tr>
<tr>
<td>Pre-exp boundary diffusion mobility</td>
<td>( B_{ab} ) (m(^3)/sec)</td>
<td>3.8 \times 10^{-12}</td>
<td>1.015 \times 10^{-12}</td>
</tr>
<tr>
<td>Activation energy for boundary diffusion</td>
<td>( Q_b ) (kJ/mol)</td>
<td>202</td>
<td>125</td>
</tr>
<tr>
<td>Pre-exp volume diffusion mobility</td>
<td>( D_{av} ) (m(^2)/sec)</td>
<td>5.9 \times 10^{-3}</td>
<td>9.54 \times 10^{-4}</td>
</tr>
<tr>
<td>Activation energy for volume diffusion</td>
<td>( Q_v ) (kJ/mol)</td>
<td>339</td>
<td>132</td>
</tr>
<tr>
<td>Work-hardening exponent</td>
<td>( k ) (MPa)</td>
<td>1181</td>
<td>3342</td>
</tr>
<tr>
<td>Work-hardening coefficient</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Experimental studies [14] indicate that an exponential PDF models the while \( \phi_n \) is well approximated by a Gaussian PDF:

\[
\phi_n(r) = \lambda e^{-\lambda r}
\]

\[
\phi_n(h) = \frac{1}{2\pi\sigma_n} \exp \left[ -\frac{1}{2} \left( \frac{h - \bar{h}}{\sigma_n} \right)^2 \right]
\]

where \( \lambda \) is the asperity radius factor, \( \bar{h} \) is the mean asperity height, and \( \sigma_n \) is the standard deviation of asperity heights. The statistical parameters \( (\gamma, \lambda, \bar{h}, \sigma_n) \) that define the surface roughness can all be obtained from a single profilometer line scan. Typical values for a TMC composite monotape are given in Table 4. It is important to realize that significant tape-to-tape variability can arise in these parameters as the droplet superheat, substrate temperature, droplet diameter, alloy composition, fiber diameter, fiber spacing, etc. are varied during the spray deposition process used to create the monotapes [51, 52]. It may therefore be possible to adjust the spray process to create monotapes with statistical parameters best suited to consolidation.

Equation (9) can be solved by substituting an initial value for the applied stress and the relative density at time, \( t = 0 \), and determining the densification rate by iterative solution of

\[
\Sigma(D^s, D^v) - \gamma \int \phi_n(h)F_c(h, r, D^s, D^v) dh = 0
\]

This can then be integrated over the next time step to obtain a new density one time step further into the process. The processing temperature enters the model either explicitly (e.g. for diffusional flow) or, more usually through the temperature dependence of the various material parameters (i.e. Young's modulus, yield strength, power-law creep exponent, etc.). Examples of these parameters for two titanium alloys were shown in Table 3. Data for many others can be found in Ref. [53].

The densification of the \( r \)-lamina, and of the \( s \)-lamina during Stage II occurs by the shrinkage of internal voids. These have been treated as uniformly sized, noninteracting (i.e. a dilute concentration of) spheres. Their collapse has been assumed to be unaffected by the presence of a fiber. The overall densification rate could then be found from the components of the macroscopic strain rate tensor, \( \dot{E}_{ij} \), within a porous body subjected to stresses, \( \Sigma_{ij} \). These are given by the gradient of a deformation potential function, \( \Phi^m \), where \( m \) represents the operative deformation mechanism (i.e. plasticity, power-law creep or diffusional flow) [14]

\[
E_{ij} = \Delta \frac{\partial \Phi^m}{\partial \Sigma_{ij}}
\]

Here, \( \Delta \) is a scalar multiplier which may depend on the loading path. In the model of Elzey and Wadley [14], Gurson et al.'s [54] potential function was used for Stage II plasticity (Doraivelu et al.'s potential function can also be used [55]), Duva's [50] potential function was used for power-law creep and a potential suggested by Ashby [55] was utilized for diffusional flow. These density-dependent potential functions are summarized in Table 2.

The principal strain rate components within each lamina can be obtained by summing the

Table 4. Statistical surface roughness parameters for surface [14]

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Symbol (units)</th>
<th>Value (units)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial density-s-layer</td>
<td>( D^s_{av} )</td>
<td>0.35</td>
</tr>
<tr>
<td>Initial density-r-layer</td>
<td>( D^r_{av} )</td>
<td>0.30</td>
</tr>
<tr>
<td>Initial height of asperity</td>
<td>( z_0 ) (m)</td>
<td>210.52 \times 10^{-4}</td>
</tr>
<tr>
<td>Mean of asperity heights of s-layer</td>
<td>( \bar{h} ) (m)</td>
<td>91.96 \times 10^{-4}</td>
</tr>
<tr>
<td>SD for asperity heights of s-layer</td>
<td>( \sigma_h ) (m)</td>
<td>39.82 \times 10^{-4}</td>
</tr>
<tr>
<td>Radius of s-layer</td>
<td>( r ) (m)</td>
<td>70 \times 10^{-4}</td>
</tr>
<tr>
<td>Asperity radii exponential factor</td>
<td>( \lambda ) (m)</td>
<td>0.0178</td>
</tr>
<tr>
<td>Areal density of asperities</td>
<td>( \gamma ) (m(^2)/tab)</td>
<td>5 \times 10^{-2}</td>
</tr>
<tr>
<td>Lineal density of asperities</td>
<td>( \rho ) (m)</td>
<td>3.87 \times 10^{-3}</td>
</tr>
</tbody>
</table>
contributions from each of the Stage II deformation mechanisms

\[ \dot{E}_i = \dot{E}_n + \dot{E}_r + \dot{E}_d. \]  

(13)

Because lateral deformations are resisted by the r-lamina, densification occurs under a constrained uniaxial compression strain state and so the densification rate \( \dot{D} = -D \dot{E}_{xx} = -D \dot{E}_{zz} \).

The effect of the fibers' presence on the densification of the r-layer has recently been examined by Duva and Crow [49]. They have shown that when the creep exponent is relatively low (\( n < 5 \)), the fiber has a relatively small effect upon the r-layer's creep densification rate, even for the highest fiber volume fraction achievable (78.5% when the fibers are in a square array touch). Since the fibers perturbation to the overall (s plus r-layer) density will be even smaller, calculations with the Duva–Crow potential will show that this effect can be safely ignored for many of the materials of interest (those which have relatively low \( n \)-values in the temperature-stress region used for consolidation).

2.2. Fiber fracture

Experimental studies have shown that significant fiber microbending and fracture sometimes accompanies the consolidation of spray deposited TMC monotapes [43]. It can be caused by matrix flow in the fiber direction [29], or on cooling after consolidation if the tooling has a lower CTE than the composite [26]. This has been shown to be most frequently caused by force concentrations that develop in regions where larger asperities contact the fibers in an adjacent monotape, Fig. 2. Using the unit cell of Fig. 2, a micromechanical model has been developed to calculate the distribution of bend stresses within the fiber and therefore determine the probability of fiber failure for a given cell. By integrating this failure probability over the distribution of cells that exist within a consolidating sample, it is then possible to determine the number of fiber fractures per unit length of fiber throughout a consolidation cycle [33].

The representative unit cell chosen for analysis consisted of a single fiber undergoing three-point bending due to forces imposed by (three) contacting asperities. An important parameter determining the response of such a unit cell is the spacing between the asperities, i.e. the length of the fiber segment in bending. The deflection (\( \nu \)) of the elastically deforming ceramic fiber in this cell can be calculated using simple beam theory [33]. From this, the stress, \( \sigma_f \), within the fiber can be determined and the probability of fracture obtained for a fiber with a known (Weibull) strength distribution. While the unit cell deflection response is relatively easy to describe [from the solution of a single nonlinear ordinary differential equation (14) given below], prediction of the overall rate of fiber fracture is more complicated because as densification occurs, the number of asperities that make contact along the length of a fiber continually

Fig. 2. The unit cell used to analyze fiber microbending/fracture [33].
increases. As new contacts are established, old bend segments become sub-divided into shorter cells that eventually become more resistant to fracture. The statistical distribution of bend segment lengths is density-dependent and it is therefore necessary to calculate the number of accumulated fracture at any time by tracking the creation, deflection and elimination of bend cells as a function of density.

Earlier fiber fracture models [33] were implemented in three parts: the unit cell response was first determined. From this, the probability of fracture for a given segment was then estimated as a function of time (or density). Finally, a Monte Carlo simulation was used to model the creation and elimination of unit cells as densification occurred. When combined they enabled prediction of the fiber deflection/damage as a function of time. Originally, results from classical indentation were again used to calculate the contact forces [33]. The recent asperity blunting FEM analysis [34, 35] now enables more precise results to be substituted. This results in a nonlinear ordinary differential equation for the rate of deflection \( \dot{v} \) of a single unit cell of length, \( l \), subjected to a densification rate, \( D(t) \) by a combination of plastic/creep asperity deformation

\[
\dot{v} - \left( -\frac{2}{1 + \xi} \right) \frac{D}{\sqrt{2\pi C(n)}} \left( \frac{1}{F(n)} \right)^{2} \sqrt{2\pi C(n)} \dot{v}^{2} + \left( 1 - \frac{D(t)}{D^*(t)} \right) k_{s}(t).
\]

(14)

The non-dimensional parameter \( \xi = 2k_{s}/k_{p} \), where the “plastic stiffness” of the asperity is \( k_{s} = 2\pi\sigma_{f}(F, + F_{m}x_{f}) \), for the plasticity mode of asperity blunting and fiber’s elastic bend stiffness is \( k_{p} = (3\pi/4)E_{f}(d_{f}^{2}/l) \), in which \( E_{f} \) and \( d_{f} \) the fiber modulus and diameter, respectively, and \( l \) is the length of fiber in the cell. The fiber deflection can be computed by integrating the differential equation (14) using the densification model [equation (1)] to determine \( D(t) \) and \( D^*(t) \). The maximum fiber bending stress \( \sigma_{f} \) is obtained from the deflection, \( v \), using a classical result of beam theory

\[
\sigma_{f} = \frac{3E_{f}d_{f}^{2}}{l^{2}}v(t).
\]

(15)

If the fiber strength distribution is described by a Weibull probability density function, the cumulative probability of fracture for a single fiber subjected to a stress \( \sigma_{f} \) is

\[
\Phi_{f}(\sigma_{f}) = 1 - \exp\left( -\left( \frac{\sigma_{f}}{\sigma_{ref}} \right)^{m} \right).
\]

(16)

Examples of the fiber properties used in the model are given in Table 5 for two types of silicon carbide monofilaments.

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Symbol (units)</th>
<th>SCS-6</th>
<th>Sigma 1240</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter ( d_{f} ) (( \mu )m)</td>
<td>140</td>
<td>100</td>
<td></td>
</tr>
<tr>
<td>Young’s modulus ( E_{f} ) (GPa)</td>
<td>425</td>
<td>400</td>
<td></td>
</tr>
<tr>
<td>Reference strength ( \sigma_{ref} ) (GPa)</td>
<td>4.5 ± 0.2</td>
<td>3.5</td>
<td></td>
</tr>
<tr>
<td>Weibull modulus ( m )</td>
<td>13.0 ± 2.1</td>
<td>12</td>
<td></td>
</tr>
</tbody>
</table>

The data for fiber strengths given in Table 5 are for pristine fibers and are assumed independent of the consolidation conditions. They assume that the aggressive chemical reactions that occur between the fibers coating and the matrix are insufficient to degrade the fiber’s strength. Experimental studies with carbon coated SCS-6 fibers [44, 57] have indicated that this is usually the case for the temperatures and processing times normally used to consolidate TMCs. In principle, if a sufficiently high processing temperature or a prolonged processing time were used, the protective coatings could then be consumed and the fiber strengths would fall precipitously [57]. Similar experiments with the TiB coated Sigma-1740 fibers [58, 59] indicate that the usually used consolidation conditions do introduce defects in the fiber and a loss in the fiber’s reference strength. Similar observations have been reported for Nextel 610 fibers [39]. In principle, this loss of fiber strength could be accounted for in the simulation by defining the strength as a function of the time temperature during processing or of the instantaneous reaction thickness. This is probably unnecessary for SCS-6 fibers because long before the fibers are significantly weakened, their interfacial sliding stress will have risen prohibitively [44] which effectively constrains the use of aggressive fiber weakening process cycles.

The final step combines the unit cell and the cell evolution models to predict the cumulative fractures as a function of density (or time) for an arbitrary process schedule. In the past, this was performed by computing the deflection (and hence the stress and probability of fracture) for each cell from the point where it was created until it was eliminated and then summing the cumulative probabilities of fracture. However, this is a very computationally intensive approach because several thousand unit cells are typically created within a reasonable representative length of fiber (say about a meter) and each of these cells then requires the solution of a nonlinear ODE.

In order to reduce the amount of computation while still capturing the process dynamics with acceptable accuracy, the concept of “influence” functions is introduced. The range of cell sizes (i.e. fiber bend segment lengths) is discretized into “bins”. All the cells within a bin are assumed to be represented by a single cell of the average normalized cell length, \( l/d_{f} \). The difference between the number of cells created (within that bin) and the number of cells eliminated (by formation of new contacts) after an increment of density then represents the remaining number of cells of that length that are deflected and
stressed and therefore susceptible to fracture. Thus, the "influence" function, \( I(D) \), for any given bin is
\[
I(D) = N_{\text{created}}(D) - N_{\text{subdivided}}(D).
\] (17)

Using the full statistical model [33], the difference functions \([I(D)\]) for 10 linearly spaced bins have been calculated, normalized by the density dependent total number of contacts \(n_c\) and are shown in Fig. 3. The range of cell \(l/d_f\) ratios selected covers the full range of those susceptible to fracture. Although higher \(l/d_f\) ratio cells exist, they are too compliant to break. Shorter cells are also present, but they are so stiff that the asperities deform and fully densify before the fibers fail. All the smoothing functions tend to zero as the relative density reaches unity because in the full density limit, subdivision eventually eliminates all of the longer fracturable cells.

The number of cells that fracture in each bin is simply determined by computing the probability of fracture for the cell and multiplying this by the cell's influence function
\[
\Delta N_i = (n_c I(D) - N_{\text{f}}(D))\Phi_i \sigma_i). \] (18)

The total number of fractures is obtained by summing \(\Delta N_i\) over all of the bins. The influence functions are controlled by monotape geometry and do not depend on the process cycle chosen. Thus, they can usually be computed just once before a series of simulations are begun. They obviously do need to be re-calculated if any of the monotape's geometric parameters are changed during a simulation study.

An important feature of the fiber fracture model is its dependence on density and densification rate. In combination with the influence functions, the density determines the number of bend cells, the distribution of cell lengths and the deformed heights of all unit cells. The densification rate (in conjunction with temperature dependent material parameters) controls the magnitude of the forces acting on the fibers. The results of the density model (for a given pressure, temperature and time) are therefore used as input to the fiber fracture model along with the applied temperature (but not the applied pressure). This coupling of two nonlinear models results in a complex dependence of the fiber damage upon variables of the process.

2.3. Reaction zone growth

At the elevated temperatures used for the consolidation of titanium matrix composites, the matrix alloys are able to react with the fiber coatings and form various reaction product layers at the interface [44, 61, 62]. If the reaction is prolonged, this eventually consumes the coating [63], reactions occur with the fiber itself [63] and eventually a loss of the fiber's strength occurs [64, 65]. For short exposures at modest temperatures, the reactions neither degrade the interface's sliding stress, nor the fiber's strength, but as the reaction product's thickness increases (beyond about 1.2 \(\mu m\) in the SCS-6/Ti-24Al-11Nb system), increases in both the fiber-matrix debond and sliding stress are observed [44]. Many TMC properties (e.g. crack growth resistance) are deleteriously affected by increases in the sliding resistance [17] and almost all are adversely affected by a loss of fiber strength. The extent of the reaction, as indicated by say

![Fig. 3. Influence functions for 10 logarithmically spaced unit cells.](image-url)
Table 6. Kinetic parameter for matrix-fiber reactions in TMCs

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Symbol</th>
<th>Ti-24Al-11Nb/SCS-6</th>
<th>Ti-6Al-4V/SCS-6</th>
<th>Ti-6Al-4V/Sigma-1240</th>
</tr>
</thead>
<tbody>
<tr>
<td>Activation energy for the reaction</td>
<td>$Q$ (kJ/mol)</td>
<td>209</td>
<td>257</td>
<td>254</td>
</tr>
<tr>
<td>Pre-exponential coefficient</td>
<td>$k_0$ (m/s$^2$)</td>
<td>$2.27 \times 10^{-6}$</td>
<td>$3.53 \times 10^{-7}$</td>
<td>$1.6 \times 10^{-7}$</td>
</tr>
</tbody>
</table>

the reaction zone thickness, is therefore an important microstructural parameter to control during consolidation.

A fundamental model for this process would involve the formation and solution of a reaction-diffusional problem. This requires a knowledge for the contiguity of the reaction surface and the diffusion coefficients for each of the diffusing species in the fiber, the matrix and in each of the reaction products formed at the interface. Unfortunately, this information is unavailable for many of the compounds that form between titanium alloys and the C/Si or TiB coatings applied to silicon carbide fibers in use today. However, experimental studies of several titanium matrix composite systems, including Ti-24Al-11Nb/SCS-6 [60], Ti-6Al-4V/SCS-6 [60,45,65] and Ti-6Al-4V/Sigma-1240 [67] have all shown that over limited ranges of temperature and time the reaction zone thickness, $\delta$, can be fitted to a simple parabolic law with respect to time

$$\delta = kt^{1/2} \quad (19)$$

where the parabolic rate constant, $k$, has an Arrhenius form

$$k = k_0 \exp \left( -\frac{Q}{2RT} \right) \quad (20)$$

In equation (20), $k_0$ is a pre-exponential coefficient, $R$ is the gas constant, $Q$ is the effective activation energy for the reaction and $T$ is the absolute processing temperature.

The reaction zone growth rate is obtained by differentiating equation (20) for $k$

$$\frac{\delta}{\delta t} = \frac{k_0^2}{2\delta} \exp \left( -\frac{Q}{RT} \right) \quad (21)$$

Data for $Q$ and $k_0$ for several systems have been collected and are tabulated in Table 6. The reaction zone growth microstructural state is not directly coupled to any of the other microstructural variables. It has important consequences for the processing of TMCs because selecting processing conditions to minimize $\delta (T, t)$ conflicts with the need to achieve near full density and a minimum number of fiber fractures per meter.

### 3. MACHINE DYNAMICS MODELS

In practice, the consolidation conditions that can be applied to a composite sample are constrained by limitations of the consolidation equipment. The pressure-temperature dynamics of the hot isostatic presses normally used for consolidation are frequently nonlinearly coupled and are not always well characterized. For example, even when no gas is added or vented, the pressure and temperature are coupled through non-ideal gas laws because of the high pressure and non-isothermal temperature conditions within the chamber [68]. The coupling depends on the furnace load (i.e. the free volume within the pressure vessel), the furnace design (particularly the ratio of heated volume to the total volume), the type of working gas, etc. Time delays also exist between commands to temperature and pressure controllers, their actuation by the machine and the establishment of their effect within the component. To fully simulate the consolidation process, a methodology is needed that allows these equipment constraints to be incorporated along with the dynamics of material evolution (as defined in Section 2).

To illustrate the approach, assume that the machine dynamics are simple in the sense that the temperature and pressure signals applied to the machine are instantly achieved in the sample, and the applied pressure, temperature and their slew rates are independent variables constrained by upper and lower bounds (more complex relationships can be easily included as needed). The machine dynamics are then defined by constraints

$$T_{\text{min}} \leq T \leq T_{\text{max}} \quad (22)$$

$$P_{\text{min}} \leq P \leq P_{\text{max}} \quad (23)$$

$$\dot{T}_{\text{min}} \leq \dot{T} \leq \dot{T}_{\text{max}} \quad (24)$$

$$\dot{P}_{\text{min}} \leq \dot{P} \leq \dot{P}_{\text{max}} \quad (25)$$

where $T_{\text{max}}$ and $T_{\text{min}}$ are the maximum heating and cooling rates, respectively, while $\dot{P}_{\text{max}}$ and $\dot{P}_{\text{min}}$ are the maximum pressurizing and depressurizing rates, respectively. Examples of temperature and pressure constraints for a representative hot isostatic press are listed in Table 7.

For TMCs, the highest soak temperature that can be used is usually limited by the material system that is being consolidated and not by the upper bound temperature of the equipment. For example, many hot isostatic presses can be operated at 1500°C or
above, whereas in the Ti-24Al-11Nb/SCS-6 system, chemical reactions between the matrix alloy and the fiber coating become so severe that ramping to 1100°C will cause unacceptable reaction product formation. The Ti-6Al-4V/SCS-6 system is even more reactive, and it is probably not feasible to exceed about 1000°C for this case.

Fig. 4. The flow chart for the dynamic simulation of TMC consolidation.
4. PROCESS SIMULATION

A simulation of a consolidation process can be thought of as an input–output device which uses models for the microstructural variables (in this case relative density, number of fiber fractures and reaction layer thickness), initial monotape geometry and material parameters, together with “admissible” input schedules (i.e. schedules that are constrained by limitations of the hot isostatic press or vacuum hot press), to predict the time-dependent microstructural evolution. The dynamic simulation of the consolidation process uses equations (1) and (2) to calculate the densities of the s- and r-laminae. The relative density of the composite is then calculated using equation (3). Since the deflection of the fibers (and hence the cumulative number of fiber fractures) is assumed to depend on \( D \), the s-layer relative density is used as an input to the fiber deflection/fracture model [equation (14)]. The rate of growth of the fiber matrix reaction zone [equation (21)] depends on neither the relative density nor fiber damage; it is only determined by the input temperature schedule and by the material parameters of the composite system (Table 6) and can therefore be calculated independently.

A flow chart for the dynamic simulation algorithm is shown in Fig. 4. This algorithm has been programmed using the matrix software MATLAB™ on a multuser IBM RS6000. A Runge–Kutta–Fehlberg (RKF) adaptive step size integration routine was used to calculate the relative density for both the s- and r-layers and the reaction layer thickness at every time step. For each time step, the plasticity contributions to densification for each of the layers was calculated before using the RKF scheme to integrate the densification rate contributions of power law creep and diffusional flow. Since the expression for the s-layer Stage I relative density due to plasticity is an implicit integral equation containing the height of the asperity, Newton’s zero finding routine was used [69]. For the Stage II s- and r-layer plasticity contributions, a standard routine for calculating the roots of the polynomial \([\Sigma - f(D) = 0]\) was used. The fiber fracture model uses the relative density as an input, and this integration of the deflection rates was performed at the completion of the density calculation for each integration step. The unit cells’ fiber deflections were computed again using Runge–Kutta–Fehlberg adaptive step size integration scheme. The RKF routines adaptively vary the integration time step for the densification, reaction zone growth and fiber deflection models to maintain the infinity norm distance between the fourth and fifth order approximations below 10⁻⁶.

The simulation required the input of numerous material parameters. Several of these parameters are functions of temperature and stress, and therefore, depend upon the temporally varying process conditions. Some parameters (e.g. the Dorn constant, \( B \), and the creep stress exponent, \( n \)) are also matrix microstructure dependent [14]. The simulations presented below have been performed using material data compiled from the literature in Tables 3, 5 and 6. The values given in the tables are representative of the processing conditions that have been extrapolated from data found in the literature. The simulation data incorporate the temperature dependence of Young’s modulus and the yield strength but do not include the temperature or microstructure sensitivity of the creep parameters. Creep constitutive models that couple the evolutionary microstructure effects with consolidation models have recently been proposed for the initially nanocrystalline microstructures created by physical vapor deposition of Ti-6Al-4V on ceramic fibers [18]. The much coarser initial grain size (2-5 \( \mu m \)) of the spray deposited material results in a less significant microstructural evolution and a weaker coupling of the creep parameters to the process conditions.

The microstructural models can be applied equally well to either hot isostatic or vacuum hot pressing. The process variables during hot isostatic pressing are the temperature and applied pressure whereas during vacuum hot pressing, they are either temperature and applied pressure or temperature and applied displacement. In the latter case, the relative density is a prescribed input function of time and this can be directly used in the fiber fracture model. The temperature, \( T(t) \), and applied pressure, \( P(t) \), schedules are assumed to be defined as time-dependent functions whose absolute values and slew rates are constrained to lie between upper and lower limits. For an (arbitrary) process cycle defined by a trajectory in a pressure, temperature, time process space, the simulation results in a path, parametric in time, along which the microstructure evolves in a “microstructural state space” whose axes correspond to \( D, N, \) and \( \delta \), Fig. 5. An “ideal” process takes the initial state in this space to a goal state that results in acceptable properties/performance. For clarity, the simulation results for each microstructural parameter shown below will be presented separately as functions of time.

5. PREDICTIONS AND EXPERIMENT

To fully evaluate the simulation’s predictive accuracy requires conducting consolidation experiments with spray deposited monotapes of known geometry and material parameters using fully defined pressure and temperature schedules. The experiments of Groves et al., [43] are the most fully characterized in the literature to-date. In these experiments, SCS-6 reinforced Ti-24Al-11Nb spray deposited monotapes were HIP densified at different plateau pressures and temperatures, and the relative density and fiber fracture density measured. Table 8. Using the HIP schedules, monotape geometry and SCS-6 fiber properties reported in Ref. [43], together with the matrix properties of Table 3, resulted in the simulated densities
and fiber fracture densities listed in the Sim. A columns of Table 8. The simulations correctly captured the trends in relative density but consistently underestimated the final relative density. Poorer agreement with fiber fracture data was observed, in part because these simulations utilize the densification model predictions.

The origin of these discrepancies is in part a consequence of the refined grain size and the metastable phases present in the spray deposited material [37]. Recent experimental works [36, 38] suggest that these finer grain size materials have creep exponents that are less than those of bulk material and exhibit higher rates of creep at the lower consolidation temperatures where coarsening is inhibited. Using a value of $n = 2$, from Ref. [36], and $B = 1 \times 10^{18}/h$ obtained by fitting measured and predicted relative densities for run HIP 02, the simulations have been repeated (column Sim. B in Table 8). The agreement between the relative densities is now much better (and might have been further improved if a fuller description of the consolidation temperature dependence of the creep properties was available). The fiber fracture trends are also now reasonably predicted with the exception of HIP 04, where the damage is underestimated. At these high temperatures, microstructural coarsening accompanies consolidation and the use of creep properties intermediate between those of the two simulations might have led to a better quantitative agreement.

These results suggest that, provided care is taken to measure or estimate the relevant model inputs, reasonable predicted trends in relative density and fiber damage are obtained. The model for the development of reaction products at the fiber-matrix interface is an empirical one. It is based upon many experimental observations of consolidated-heat treated samples, and is independent of densification or fracture. Thus, provided kinetic data for the range of consolidation temperature/times are used, reasonable values and trends for this predicted parameter would be expected.

6. TMC CONSOLIDATION SIMULATION

The simulation methodology developed above can now be used to investigate the dynamic response of TMC monotape preforms during their transient consolidation and to explore the (often) complex interrelationships between process path, monotape geometry, fiber-coating-matrix system properties and the resulting microstructural state of the composite. These are investigated in a systematic fashion by first examining the relative importance of the various densification mechanisms. The effects of changing the final temperature and pressure are then investigated. Insight into the consequences of using a different matrix alloy or fiber type, are assessed next. Finally, an analysis of the monotape geometry is performed to identify the parameters that should be controlled (or ideally optimized) during the spray deposition process in order to maximize the "processibility" of a candidate TMC system.

6.1. Densification mechanism contributions

Three mechanisms of deformation (plasticity, power law creep and diffusional flow) potentially contribute to the densification of composite monotapes. Studies of alloy powder densification have

<table>
<thead>
<tr>
<th>Schedule</th>
<th>Temp. (°C)</th>
<th>Press. (MPa)</th>
<th>Exp. Sim. A</th>
<th>Sim. B</th>
<th>Exp. (m⁻¹)</th>
<th>Sim. A (m⁻¹)</th>
<th>Sim. B (m⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HIP 01</td>
<td>825</td>
<td>50</td>
<td>0.894</td>
<td>0.7807</td>
<td>0.8210</td>
<td>138.9</td>
<td>223.1</td>
</tr>
<tr>
<td>HIP 02</td>
<td>900</td>
<td>50</td>
<td>0.958</td>
<td>0.8183</td>
<td>0.9438</td>
<td>56.3</td>
<td>348.6</td>
</tr>
<tr>
<td>HIP 03</td>
<td>900</td>
<td>100</td>
<td>0.975</td>
<td>0.8793</td>
<td>0.9921</td>
<td>135.4</td>
<td>600.2</td>
</tr>
<tr>
<td>HIP 04</td>
<td>975</td>
<td>50</td>
<td>0.979</td>
<td>0.8006</td>
<td>0.9999</td>
<td>40.4</td>
<td>150.3</td>
</tr>
</tbody>
</table>
revealed that in general plasticity dominates densification at high pressures and low temperatures whereas diffusional flow is preferred at high temperatures and lower pressures [70]. The relative importance of these mechanisms is therefore likely to be a sensitive function of the process path for each alloy system. To investigate this, a representative TMC system consisting of a Ti-6Al-4V matrix (with the properties given in Table 3) and an SCS-6 silicon carbide fiber (with the properties given in Tables 3 and 6) has been chosen as a baseline system for detailed studies. The monotapec geometry was specified by the parameters in Table 4 and the densification contributions of each of the three densification mechanisms were then calculated for the process cycle shown in Fig. 5(b). For this cycle, a 1 MPa pressure was instantaneously applied at time $t = 0$, followed by temperature ramping at a rate of 1600°C/h to a constant plateau value of 800°C. As soon as the plateau temperature was reached, the pressure was increased at 40 MPa/h to a constant plateau pressure of 100 MPa. Figures 6(a) and (b) show that the densification rate is a sensitive function of temperature, pressure and the relative density and varies significantly with time. Note the rapid increase in density when the temperature reached 600°C (while the pressure remained at 1 MPa) and the later (after about 40 min) increase in densification rate as the pressure increased through 100 MPa.

Figure 6(a) shows that the dominant deformation mechanism throughout the cycle was power law creep. Once the temperature reached or exceeded ~600°C, power law creep was the only densification mechanism. The increases in densification rate correspond to the activation of this mechanism either by an increase in temperature or applied pressure. The power law creep contributions of the s- and r-layers to densification varied as the density increased, Fig. 6(b). The s-layer was totally responsible for the early densification ($D < 0.85$); whereas the r-layer only began to significantly contribute to the densification after the s-layer exceeded a density of 0.9. This arises because at the start of densification, the initial relative density and (thus the flow resistance) of the r-layer is much higher than that of the s-layer. The r-layer densification begins to significantly contribute to the composite densification only once the s-layer’s density is comparable to that of the r-layer. When the overall density reaches about 0.9, both layers roughly contribute equally to densification.

A small (7.4%) contribution to densification from plasticity was observed during the initial heating stage of the process, Fig. 6(a). This occurred when the contact stresses (at the small number of contacts supporting the applied load) were very high and the temperature was still too low for creep. Simulations reveal that either increasing a matrix system’s creep resistance or decreasing its yield strength promotes the importance of the plasticity mechanism. However, its contribution is almost always smaller than might at first be expected. This is because the rapid growth of contact area together with the high formation rate of new contacts usually lowers the contact stress rapidly as the density increases and eliminates any further possibility of yielding unless the pressure increases. Even if the pressure is increased, a simultaneous increase of temperature at the rates typically encountered often activates high creep rates before the conditions for plasticity can be satisfied. In the Ti-6Al-4V system, plasticity only becomes a significant mechanism when the relative density is low, the temperature is < 600°C and the applied pressure is high. It will be shown later that these conditions are precisely the ones that also promote fiber bending/fracture and in general need to be avoided.

It is also clear from Fig. 6(a) that no significant densification from diffusional flow occurred in the Ti-6Al-4V matrix system, even when the temperature reached 800°C. This again is a consequence of the large power law (i.e. dislocation) creep contribution to densification. In the relatively coarse grain size Ti-6Al-4V found in spray deposited monotapecs, power law creep is the dominant high stress creep mechanism in the 600–800°C temperature range [38]. Diffusional flow contributions become more important for smaller grain size materials (e.g. as produced by vapor deposition), or at higher temperatures and lower stresses [53]. However, it will be shown later that if the temperature were increased, and the pressure decreased, in order to promote a diffusional flow

![Fig. 6. Densification mechanism and layer contributions for a representative consolidation path. (Note a 1 MPa pressure was applied at $t = 0$ throughout the temperature ramp.)](image-url)
contribution to densification, a thick reaction forms between the fiber’s coating and the matrix before it can be consolidated to full density. In order to avoid this, conditions are almost always chosen that result in insignificant contributions of diffusional flow to consolidation (unless reaction inhibiting coatings are developed for the fibers or the matrix grain size can be reduced to enhance boundary diffusional creep). For the Ti-6Al-4V/SCS-6 system, the simulations reveal that power law creep is the most important densification mechanism, and process cycles (or microstructures) that promote it are likely to result in the best composites.

6.2. Process variable effects

There are four independent variables that define a consolidation process cycle: the temperature, \(T(t)\), the pressure, \(P(t)\), and their rates, \(T'(t)\) and \(P'(t)\). The magnitudes of these quantities (together with their phase relationship) control the outcome of processing.

6.2.1. Pressure-temperature phasing. Consider the baseline Ti-6Al-4V/SCS-6 system (as defined in Section 5.1) subjected to three different process cycles (S1, S2 and S3), Fig. 7. Cycle S1 applies a pressure of 100 MPa before increasing the temperature at 850°C, cycle S2 applies pressure and temperature simultaneously, while cycle S3 applies 1 MPa at \(t = 0\), ramps the temperature to its plateau value and then increases pressure until full density is reached. Figure 7 shows the effect of these three cycles upon the temporal evolution of fiber fracture, relative density and the fiber–matrix reaction zone thickness. An ideal process would have resulted in little or no fiber fracture, a relative density of unity and insufficient reaction at the fiber–matrix interface to increase the sliding stress (say less than about 0.7 μm).

From Fig. 7, the S3 cycle (heating applied before pressurization) is seen to be the most successful of the three processes; the sample attained a full density, had the least number of fiber fractures and incurred only 0.3 μm of reaction product. From Fig. 7(b) each of the three cycles is seen to result in near theoretical density, but the path by which this was reached was different for each of the cases analyzed. Figure 7(c) shows that the final reaction product thickness for the S1 cycle is significantly less than that of either the S2 or S3 cycles because it experienced the smallest integrated thermal exposure. Though near theoretical density, acceptable reaction product thicknesses were achieved for all cycles, it is clear that applied pressure after the component reaches its final temperature reduces the fiber damage (at the modest expense of a slightly larger reaction zone thickness) and is the preferred method of processing.

Insight into the reasons for the smaller number of breaks during the S3 cycle can be obtained by comparing the evolution of fiber deflections and bend stresses for representative cells in the fiber cell length distribution, Fig. 8. The stresses for the S3 process at any time, are seen to be always less than those of both the S2 and S1 processes. Recall that it is the ratio of the matrix deformation resistance to the stiffness of the fibers that governs the bend cell deflection and thus controls the fiber stress. The fiber’s stiffness is controlled by its (length)\(^3\), its diameter and its weakly temperature-dependent Young’s modulus [equation (15)], and is therefore more or less independent of both the temperature and the pressure schedules used for processing. However, the matrix deformation resistance decreases with temperature and so does depend on the process schedule. Figure 8 shows that fiber deflections are reduced as one increases the temperature at which a given pressure is reached (i.e. by reducing the matrix asperity contact flow resistance). The bend cell stresses are therefore process path dependent and if the pressure is either applied before the temperature, as in Fig. 8(a), or simultaneously with the temperature, as in Fig. 8(d), the fiber deflections of most unit cells are higher, and this increases the fiber stress and thus the probability of fiber fracture.

Other factors are also important contributors to the fiber failure process. For example, a comparison of the fiber fracture data of Fig. 7(a) with the cell
deflections for the S1 and S2 cycles in Figs 8(a) and (d) reveals, at first sight, an apparent inconsistency: during the first 50 min of processing, the cell deflections/stresses of the S1 cycle exceed those of the S2 process, yet the number of S2 fractures greatly exceeds those of the S1 process, Fig. 7(a). However, recall that the overall fracture probability is found by summing the individual fracture probabilities for each unit cell in the cell length population. The fiber fracture probability for the fraction of the cell population of a given length is computed by multiplying the probability that a fiber of that length will fracture with its influence function (which is the probability that cells of that length exist, Fig. 3). Equation (14) indicates that the cell deflection and therefore the fracture probabilities for each length cell depend on the densification rate, while Fig. 3 shows that the influence functions are dependent on the density. Thus, although the fiber deflections are higher for the S1 cycle, its lower density and densification rate during the first 50 min of consolidation results in the existence of a smaller fraction of fracturable cells and therefore less damage.

Another, at first surprising result is seen later, at about 150 min into the process. In this case, increasing the temperature during cycle S1 is seen to cause very significant fiber fracture even though the pressure remained constant. Recall that increasing the temperature both softens the asperities and increases the rate of densification. The temperature dependent softening decreases the contact forces and the cell deflections, whereas the high rate of densification will tend to increase them. This latter effect dominates for a short time during temperature ramping, and in conjunction with the simultaneous increase in the population of fracturable cells associated with the rapid increase of density, results in an increased amount of fracture.

6.2. Rate effects. The results above indicate that the best composites are to be expected from processes in which the temperature is raised prior to the application of pressure. For cycles in which the temperature is applied before the pressure, the majority of fiber damage occurs when the densification rates are the highest, i.e., during the elevated temperature pressurization stage of the cycle, Fig. 7. To systematically investigate the effect of varying the temperature and the pressure rate upon the density and fiber fracture probability, a series of simulations were conducted where temperature was applied before pressure using the Ti-6Al-4V/SCS-6 baseline system. The pressurization rate was varied between 10 and 80 MPa/h at plateau temperatures of between 450 and 900°C. These results were then used to create damage and density maps in a pressurization rate-temperature space for various times after the start of the consolidation cycle, Fig. 9.
The maps show that the density increased monotonically as either the temperature, the pressurization rate or the consolidation were increased. Fiber fracture on the other hand exhibited a much more complex relationship with these process variables. It is evident that increases in pressurization rate usually increase the damage the higher densification rate and reduced time for asperity flow enforce larger fiber deflections. However, the effect of temperature is less intuitive. At intermediate temperatures, ~700°C, a maximum is seen in the damage for a fixed pressurization rate and time. The damage also increases rapidly during the early stages of the process. These two effects can be rationalized by recalling that the rate of fiber bending increases with densification rate if the asperities are unable to inelastically deform (e.g. at low consolidation temperatures). Both the densification rate and the rate of asperity creep increase as the temperature increases. Below ~700°C, the increasing rate of densification with temperature promotes fractures, whereas above about 700°C, the decreased deformation resistance of the asperities is sufficient to compensate for the higher rate of densification. The net effect causes the deflections and stresses of each $l/d_t$ ratio unit cell to decrease as the temperature increases and the damage is reduced.

The maps reveal an interesting strategy for densification without fiber fracture. High pressurization rates at low temperatures are seen not to be damaging to the fibers during the first few (10-20) minutes of consolidation and they accomplish some densification. However, as the temperature increases towards 700°C, the fiber stresses increase, and it is necessary to reduce the pressurization rate to a few MPa/h to avoid fiber damage. Once the temperature rises above about 750°C, the pressurization rate can then be increased again. As full density is approached, the probability of fiber failure falls almost to zero at temperatures above 800°C and so very high pressurization rates could then be safely applied to finish consolidation. This type of consolidation process is also likely to result in the smallest integrated thermal exposure and will therefore lead to a reduced reaction zone thickness compared with many other schedules.
that also attain full density and minimal fiber damage.

6.2.3. Pressure–temperature plateau. The most promising (least fiber microbending/fracture) approaches for fully consolidating TMC monotapes increase pressure (subject to the rate constraints above) to a plateau value only after the temperature has reached its plateau value. The results above suggest that the plateau pressure and temperature used during a consolidation process of this type are likely to have a significant effect upon the composite’s microstructural state (relative density, fiber microbending stress/fracture, reaction zone thickness). To investigate this, two series of simulations were conducted. For the first, Fig. 10, the temperature was ramped (at 1600 °C/h) to a preset plateau value of either 700, 800 or 900 °C and a pressure of 100 MPa was then applied at a rate of 40 MPa/h. For the second series, Fig. 11, the temperature was raised to 800 °C and the pressure then ramped to 25, 50 or 100 MPa at 40 MPa/h. The material system and the monotape geometry were the same as above (the Ti-6Al-4V/SCS-6 baseline system). The simulations were continued for each test until either the relative density reached 0.99 or until 660 min of processing time had elapsed.

Figure 10 shows the marked effect of the plateau temperature upon the final microstructural state of this composite system. Consolidation at 700 °C and 100 MPa successfully controlled fiber–matrix reactions, but resulted in ~700 fiber breaks per meter and failed to achieve the target relative density even after an 11 h consolidation cycle. Increasing the plateau temperature to 900 °C (S3 cycle) overcame the fiber microbending problem while allowing the target density to be reached in about 90 min (before the pressure had reached its plateau value). Even though the reaction rate between the fiber and matrix was very rapid at this high temperature, the short processing time required for densification resulted in only a doubling (to ~0.4 μm) of the reaction zone thickness. A less satisfactory result was obtained at 800 °C. Although the target density was reached (within 3 h) without an appreciable increase in reaction zone thickness (because the shorter consolidation time almost fully offsets the increased temperature), approximately 80 fiber breaks per meter are predicted.

Reducing the pressure while maintaining the 800 °C temperature plateau, does not significantly improve matters, Fig. 11. Reducing the plateau pressure from

![Fig. 10. The effect of varying the maximum consolidation temperature for a fixed maximum pressure (100 MPa) using the baseline Ti-6Al-4V/SCS-6 system.](image)

![Fig. 11. The effect of varying the maximum consolidation pressure for a fixed maximum temperature (800 °C) using the baseline Ti-6Al-4V/SCS-6 system.](image)
100 to 50 MPa fails to reduce the number of fiber fractures whilst it doubles the reaction zone thickness (because of the longer time at 800°C required to reach the target density). Similar amounts of fracture arise because the densification rates are the same during the "ramp" stage of the pressure schedule, and since the fiber damage model is very sensitive to the initial part of the process, almost the same amount of fiber damage results. Although very low pressures (25 MPa) are seen to be successful at reducing damage, they require excessively long processing times to reach full density and incur unacceptable levels of fiber-matrix reaction.

The simulations of Section 5.2 lead to the conclusion that composites with near theoretical density, acceptable reaction zone thickness, and with little or no fiber fracture can be successfully processed from spray deposited Ti-6Al4V/SCS-6 monotapes. The best process cycles for this always apply the temperature before the pressure is ramped. To avoid excessive fiber bending, the rate of pressurization must be kept below a temperature-dependent critical value. This value rises rapidly as the consolidation temperature is increased to 800°C and at 900°C the full pressurization rate capabilities of a modern hot isostatic press can be safely exploited to fully densify components in less than 2 h. The short processing time partially offsets the higher fiber-matrix reaction rate at 900°C and enables acceptably small reaction zone thicknesses to still be obtained.

6.3. Material effects

The dynamic response of the TMC system analyzed above originates in the pressure- and temperature-dependent inelastic flow characteristics of the Ti-6Al-4V matrix, the diameter, modulus and strength of the SCS-6 fibers and the kinetics of the chemical reactions between the fiber's coating and the surrounding matrix. An acceptable process cycle could be designed for this system because of the unique balance of fiber-matrix properties for this system. Several other matrix alloys and fiber types are currently being explored for the synthesis of titanium matrix composites. Changing either the matrix alloy or the fiber type will result in a different combination of system properties that might be expected to impact the success of the process. The dynamic simulations afford a straightforward methodology to investigate this issue and provide insight into the material system factors that govern the processibility of candidate TMC systems.

6.3.1. Matrix. To illustrate the significance of the matrix upon microstructural evolution, the mechanical properties of Ti-24Al-11Nb (given in Table 3) have been substituted for those of Ti-6Al-4V. Ti-24Al-11Nb is an $\alpha_2 + \beta$ intermetallic alloy with a better high temperature creep resistance than Ti-6Al-4V [36]. Figure 12 shows the effect of changing the plateau temperature upon the relative density, fiber fracture probability and reaction zone thickness. The enhanced resistance of the matrix to creep is manifested in a reduced relative density compared to Ti6Al4V (compare Fig. 12 with Fig. 10). Using a 100 MPa plateau pressure, a target density of 0.99 is only reached in 180 min at 1000°C (cycle S3) in the Ti-24Al-11Nb system [Fig. 12(b)]. While this cycle successfully limits fiber fracture [Fig. 12(a)], it results in about a 1.2 µm thick reaction product [Fig. 12(c)] which is unacceptable for this system since it corresponds to the thickness at which the interface sliding stress begins to increase [32]. Reducing the plateau temperature to 900°C (cycle S2) to retard the interfacial reaction, fails to achieve an acceptable microstructure because the target density is not achieved even after 660 min of processing (by which point the interfacial reaction zone had grown to a thickness of ~1.0 µm and excessive fiber fracture had occurred). Reducing the pressure at 900°C, Fig. 13, fails to significantly reduce the fiber fracture problem and would require the use of extended processing times (with an unacceptable reaction zone thickness) to attain the target density.

These results clearly indicate that the matrix system has less processibility than one using the Ti-6Al-4V alloy. It stems from the increased resistance of the matrix to creep which forces the use of higher
consolidation temperatures to densify the composite. While this enables densification without fiber fracture, it results in the formation of unacceptable thick fiber–matrix reaction products (even though the reaction rate in Ti-24Al-11Nb is less than that in the Ti-6Al-4V system). Fine tuning the pressurization rate during pressure ramping may offer an opportunity to reduce the fiber fracture problem at lower temperatures, but the high temperature/pressures required for complete consolidation almost always result in an unacceptable reaction product thickness. These results help to explain observations in the literature where relatively good (close to theoretical) performance has been obtained for Ti-6Al-4V/SCS-6 composites but much lower than expected strength has often been found in the Ti-6Al-4V/Sigma 1240 system. In view of the results above, it is likely that all efforts to use matrices with creep resistances significantly greater than Ti-6Al-4V will be susceptible to these types of problems. The solution may again be to reduce the fiber–matrix reaction rates by developing fiber coatings that inhibit matrix–fiber interdiffusion at the high temperatures needed for densification.

It is clear from the above that the microstructural states developed during a consolidation cycle depend upon mechanical properties of the matrix. For the baseline Ti-6Al-4V/SCS-6 system power law creep has been shown to be the dominant densification mechanism whilst fiber fracture has been shown to be very sensitive to the densification rate which also depends on the matrix creep behavior. The relative density or number of fiber fractures per unit length of fibers is therefore likely to depend strongly upon the material parameters characterizing creep, i.e. the matrix material’s creep exponent, n, and the activation energy for creep, Q_c.

6.3.2. Fiber. The elastic bend stiffness and the strength of the fiber in a candidate TMC system both play important roles during process-induced fiber fracture. To investigate the significance of this, the properties of Sigma 1240 fibers have been substituted for those of SCS-6 fibers and the simulations of Figs 10 and 11 repeated. Although SCS-6 and Sigma 1240 fibers are both produced by similar chemical vapor deposition processes, the resulting fibers have different diameters and strengths and exhibit different reaction kinetics with the Ti-6Al-4V matrix (because the Sigma 1240 fiber is TiB coated).

Figure 14 shows the effect of varying the plateau temperature for the Ti-6Al-4V/Sigma 1240 system.
The density, Fig. 14(b) obviously is unaffected by the change of fiber (and is shown only to simplify interpretation of the other microstructural states). This fiber is seen to exhibit significantly more fiber fracture than the SCS-6 system. Even at the highest plateau temperature of 900°C, over 300 fiber breaks per meter of fiber are predicted. Thicker reaction products are also observed at each temperature. Reducing the plateau pressure, Fig. 15, does slightly reduce damage, but at the expense of a significant lowering of the density and a further increase in the reaction zone thickness. These differences in behavior illustrate the sometimes extreme nonlinear dependence of the microstructural states upon the input material parameters. In this case, relatively small changes in fiber properties (particularly the reduction of the fiber diameter from 140 to 100 μm) greatly increase the susceptibility to fiber damage and therefore adversely affects processibility.

6.4. Monotape geometry

The surface roughness of spray deposited monolantes determines the form of the cell influence functions and must therefore affect the processibility of all composite systems. The roughness is controlled by the conditions used for spray deposition (e.g. droplet diameter, velocity, superheat and fiber spacing) which govern the degree of droplet spreading before freezing and, therefore, the flatness of the as-deposited surface [8, 51, 52]. To this point, all of the simulations have used a surface roughness defined by the experimentally measured parameters of Table 4. Simulation trials with the model reveal that the mean asperity height, \( h_0 \), has little effect upon processibility. The asperity density has a stronger effect and damage is reduced if the number of asperities is either increased or decreased from the value used above. However, the most critical parameter is found to be the standard deviation (\( \sigma_h \)) of the asperity height distribution which controls the form of the influence functions \( f(D) \) used in the fiber fracture model.

To investigate the effect of the surface roughness variability, additional simulations were performed using asperity height standard deviations of 30, 40 and 50 μm, while keeping all other material parameters the same as those used for the benchmark Ti-6Al-4V/SCS-6 system. This required the computation of new influence functions for the 30 and 50 μm standard deviation cases. Figure 16 shows the

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Fig. 15. The effect of varying the maximum consolidation pressure for a fixed maximum temperature (800°C) using the new Ti-6Al-4V/Sigma-1240 system.

Fig. 16. The effect of varying the standard deviation of the monotape's surface roughness.
effect of \( \sigma_\text{ref} \) upon the microstructural state evolution for a process cycle in which the temperature is fully ramped prior to loading. The initial layup density decreases with increasing \( \sigma_\text{ref} \) because the height of the largest asperities defined the initial density (taken for convenience to be \( h + 3\sigma_\text{ref} \)). The time to reach a relative density of 0.99 increased slightly as \( \sigma_\text{ref} \) was increased because a higher fraction of the asperities suffered bigger deformations with a larger geometrical constraint [37, 38]. The increased time also resulted in slightly larger interfacial reaction product thicknesses.

Figure 16 shows that the most significant effects of \( \sigma_\text{ref} \) are seen in the fiber fracture behavior. Reducing \( \sigma_\text{ref} \) from the 40 \( \mu \text{m} \) value used for the benchmark calculations to 30 \( \mu \text{m} \) almost completely eliminates the fracture problem and, therefore, greatly enhances the "processibility" of this and the other composite systems. The origin of this strong effect lies in the evolving distribution of cell lengths, Fig. 17. When the asperity height distribution is small, fewer cells of a length susceptible to fracture are created in the low relative density region where the chances of fiber fracture are highest. As the density evolves, more cells are created with smaller aspect ratios. These cells are much stiffer and are therefore less likely to fracture. The surprisingly strong effect shown in Fig. 16 results from a cascading of several nonlinear processes (influence function dependence on \( \sigma_\text{ref} \), cell length dependence of the bending stress, the Weibull nature of fiber strength, etc.) and reinforces the importance of a modeling approach for improving the processing of this class of materials.

6.5 Materials selection criteria

The results above reveal a strong (and sometimes highly nonlinear) sensitivity of the predicted states to input material and geometric parameters. This can be used to elucidate general guidelines for selecting materials of high processibility. The "processibility" of a system (i.e. the ability to fully densify it with

![Diagram](image_url)

Fig. 18. A schematic illustration showing how an increase in a material or monotape parameter effects the processibility reinforced titanium composite.
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minimal reactions and little or no fiber breakage) can be improved by increasing some properties of the system and decreasing others, Fig. 18. Compared to a baseline system (Ti–6Al–4V/SCS-6), processibility can be improved by increasing $m$, $\sigma_{eff}$, $E_f$, $d_f$, $B(T)$ and $n$. Either increasing or decreasing the number of asperities/$m$ ($\rho$), from the 3500–4000/$m$ range of the baseline system also improves the processibility. Figure 18 also shows that the likelihood of successfully processing a composite decreases as $Q_{as}$, $\sigma_f$ and $\sigma_f(T)$ are increased. The analysis reveals that many materials become potentially processible if $\sigma_f$ is reduced or if the fiber strength $\sigma_{eff}$ is increased from the values used for the baseline system.

7. DISCUSSION

In mathematical terms, the general features of this class of process simulation problems are a set of coupled, nonlinear ODEs in the microstructural states with time-varying material and process parameter inputs. The parameters which represent material characteristics and geometric features of the processing problem may not have deterministic values, but rather may be described using a suitable probability density function. When this is the case, the representative volume elements (or unit cells) making up the continuum must exhibit a stochastic distribution of responses to a given process history. The number of models, corresponding to the number of microstructural variables, and their statistical complexity are then constrained only by limitations on computational resources. The simulation approach pursued here was based on the solution of 12 coupled ODEs (rather than PDEs or finite element analysis) as a consequence of this computational restriction. The simulation, or “forward problem” has sought to obtain the microstructural state variable as a function of time by integrating the set of ODEs for a given process machine constrained process history.

In cases where three microstructural variables (or less) are used to describe the material’s state, the evolution of microstructure may be viewed as a trajectory in a space whose axes are the microstructural variables, Fig. 2(a). Since each microstructural variable is evolving as a function of time, the plot has axes of reaction zone thickness, number of fibers fractured per meter and relative density and is parametric in time. An optimal trajectory in this space would be constrained to the relative density axis, implying no fiber damage or interfacial reaction. Material systems that approach this behavior are the most processible. In reality this is unlikely for any TMC system; in practice, some level of reaction always occurs at the high temperatures needed to avoid highly deleterious fiber microbending/fracture.

Defining acceptable limits for the microstructural variables must ultimately depend on the property/performance requirements for the as-processed material (or a final component made from it). This requires microstructure state-property relationships that predict the dependence of mechanical (or other) properties on the simulated microstructural (and other) variables. For the case of TMC consolidation processing, the influence of porosity on matrix mechanical properties has been extensively studied [54, 49, 50]. Models have also been developed that capture the influence of the number of fiber breaks (and residual fiber microbend stresses) on the tensile and creep rupture strength [17, 21]. Some limited progress has been made in determining the relationships between interfacial reaction growth and mechanical properties [44], but considerably more work is needed in this area. Structure–property relationships of this type allow the formulation of realistic objectives for the microstructural evolution, and thus the potential for the setting up of an “inverse” problem that searches for the process paths that satisfy such objectives.

8. CONCLUSIONS

Micromechanical models of densification and fiber bending have been combined with empirical kinetic relationships between reaction product formation and temperature/time to simulate the evolution of the relative density, number of fiber fractures$/m$ and the reaction product thickness in TMCs manufactured via the hot isostatic or vacuum hot pressing of spray deposited monotapes. These microstructural aspects combine with other less process sensitive parameters (e.g. fiber modulus, volume fraction or strength, matrix modulus or strength, etc.) to control the performance of TMC components manufactured by this process. Detailed simulations conducted with the model have separately investigated the effects upon the microstructural evolution of process schedule, material system properties and monotape geometry. The Ti–6Al–4V/SCS-6 system has been found to be highly processible in the sense that full densification can be achieved from sprayed monotapes using process cycles that cause little or no fiber fracture and only slight reaction between the fiber coating and the matrix alloy. This arises because at temperatures of ~850–900°C, the matrix has a low flow stress facilitating rapid densification without introducing large bending stresses. The modeling approach has been used to provide qualitative guidelines for selecting materials and monotapes that are likely to result in good processibility. While this study has focused on the consolidation processing of plasma spray-deposited monotape preforms, many of the qualitative trends with material properties and process parameters are also likely to apply to other TMC preform types.

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