1 of 1

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NUMERICAL SIMULATIONS OF CREEP IN DUCTILE-PHASE TOUGHENED INTERMETALLIC MATRIX COMPOSITES

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ABSTRACT

Analytical and finite element method (FEM) simulations of creep in idealized ductile-phase toughened intermetallic composites are described. For these strong-matrix materials, the two types of analyses predict similar time-independent composite creep rates if each phase individually exhibits only steady-state creep. The composite creep rate becomes increasingly higher than that of the monolithic intermetallic as the stress exponent of the intermetallic and the volume fraction and creep rate of the ductile phase increase. FEM analysis shows that the shape of the ductile phase does not affect the creep rate but may affect the internal stress and strain distributions, and thus damage accumulation rates. If primary creep occurs in one or both of the individual phases, the composite also exhibits primary creep. In this case, there can be significant deviations in the creep curves computed by the analytical and FEM models. The model predictions are compared with data for the $\text{Nb}_5\text{Si}_3/\text{Nb}$ system.

INTRODUCTION

The use of a ductile phase to toughen brittle intermetallics has been examined widely in the past several years (*e.g.* [1,2]) as a means of developing advanced materials for high temperature structural use. The focus of the research to date on these ductile-phase toughened (DPT) materials has been on improving low temperature toughness. The high temperature deformation behavior of these intermetallic matrix composites (IMCs) has received only limited attention, *e.g.* [3-5]. There are two features of deformation in these DPT IMCs that separate them from the well-studied case of metal matrix composites (MMCs): (1) both phases undergo time-dependent deformation, and (2) the matrix is likely to be the stronger, or more creep resistant, phase. The purpose of the work presented here was to begin exploring time-dependent deformation of discontinuously reinforced IMCs using numerical techniques. These efforts supplement earlier numerical studies in which either one phase [6,7] or both phases [4,8-11] deform by creep.

The numerical models used in this study, both analytical and finite element method (FEM), rely upon a continuum description of deformation in each phase. As discussed by Dragone and co-workers [6,7] for creep of metal matrix composites (MMCs) with elastic reinforcements, this simplification provides accurate predictions of deformation for some systems but not for others. The situation for composites in which both phases undergo creep is less clear. In any case, solution of the continuum problem is a useful first step in understanding creep of these ductile two-phase materials.

The majority of simulations performed in this study were for discontinuous fiber composites, though limited results for spherical reinforcement geometries are presented. Efforts were focused on idealized DPT composites, for which the "strong" matrix has the lower intrinsic creep rate. These results are compared with those for conventional MMCs, in which the "weak" matrix creeps at a faster rate than the reinforcement. One major goal was to determine quantitatively how severely the creep resistance of strong intermetallic materials is degraded by forming a composite with a ductile, creep-weak phase. In addition, this research addresses the usefulness of relatively complex FEM analyses compared with a simple analytical approach. Finally, the predictions of these continuum models are compared with preliminary data for the steady-state creep of $\text{Nb}_5\text{Si}_3/\text{Nb}$ composites [5].

NUMERICAL METHODS

Following many previous numerical investigations [6,8,12,13], simulations were performed for uniaxially loaded, idealized composites consisting of a regular array of discontinuous cylindrical fibers or spheres embedded in a continuous matrix. Due to the regularity of this geometry, only a “unit cell” of material was considered. This unit cell consists of one fiber or sphere that, in two dimensions, is embedded within a cylinder of the surrounding matrix in proportions to match the volume fractions actually present in the idealized composite. Perfect bonding between the two phases was assumed. Thus, the important effects of cavity formation or interphase sliding [4,7,8] were not simulated. More complete descriptions of the unit cell approximation are available elsewhere [6,8,12,13].

As discussed in detail elsewhere [14], the idealized composite geometry and uniaxial tensile loading allowed for a two-dimensional axisymmetric FEM model. The reinforcement volume fractions were varied from 21.6 to 51.2%. For the short fibers, length-to-diameter ratios of 5.0 were used in all of the simulations for both the fiber and the unit cell. The well-established “unit cell” boundary conditions were employed to ensure continuity during deformation between unit cells in a repeating array [6,8,12,13]. The FEM calculations were performed using the implicit, two-dimensional, non-linear, solid mechanics code NIKE2D [15]. A constant applied stress was simulated by continuously decreasing the applied force during the simulation to account for the reduction in the radius of the deformed mesh. In addition to elastic deformation, both of the phases in the composite were assumed to creep according to the equation [16]:

$$\epsilon_{cr} = A (\sigma_{eff})^n t^m, \quad (1)$$

where ϵ_{cr} is the von Mises effective creep strain, σ_{eff} is the von Mises effective stress, t is time, n is the stress exponent, and A and m are constants. Transient creep is simulated by a time exponent, m , other than unity. For the case of $m = 1$, or steady-state creep, the strain rate reduces to the familiar Norton power law.

In addition to FEM simulations, a simple analytical model of composite creep based on the work of Bullock *et al.* [9] and Tanaka *et al.* [11] was employed in this study. This model assumes strain compatibility between the phases and uniform stress and strain states within each phase. For each phase, i , the total strain, ϵ_i^{tot} , is:

$$\epsilon_i^{tot} = (\sigma_i/E_i) + A_i \sigma_i^{n_i} t^{m_i}, \quad (2)$$

where σ is the stress and E is Young's modulus. From strain compatibility,

$$\dot{\epsilon}_w - \dot{\epsilon}_s = 0, \quad (3)$$

where the subscripts w and s refer to the weak and strong phases. Differentiating (2) with respect to time for each phase and substituting into (3) yields a nonlinear expression for the two unknowns: the stresses in the strong and weak phases, σ_s and σ_w . At each time step in the simulation, these stresses can be computed using Newton's method [17], with the rule-of-mixtures constraint:

$$V_s \sigma_s + (1-V_s) \sigma_w = \sigma_{app}, \quad (4)$$

where V_s is the volume fraction of the strong phase and σ_{app} is the applied stress. Once σ_s and σ_w are determined for the current time step, the increment in total strain for each phase (and thus the composite) can be computed by substitution into the incremental form of eq. (2). Integrating

these incremental results over all time steps in the simulation gives the stress in each phase and the total composite strain as a function of time.

NUMERICAL RESULTS AND DISCUSSION

To assess some of the behavioral trends, computations for model composites first were performed. To simplify the calculations, the two phases were given identical stress exponents of 4.9. The creep rate in each phase was varied by varying the constant A . The volume fractions of the two phases also were varied, as was the position of the strong phase: strong matrix, *i.e.* DPT IMCs, or weak matrix, *i.e.* MMCs. The focus was on steady-state creep but preliminary calculations also were performed for primary creep, $m < 1$.

For the constant applied stress conditions simulated, both models predict linear composite creep strain vs time curves when $m = 1$ in both phases. The presence of two phases with different individual steady-state creep rates (due to differences in A) did not cause non-linearity of the strain-time curves. This finding differs from that for a steady-state creeping matrix with discontinuous elastic reinforcements, where non-linearity in the strain-time curve initially occurs due to the redistribution of internal stresses [6,10]. In the present study, both models show that the (non-uniform) stress state developed immediately after loading remains essentially unchanged with further time or strain. The result of this constant stress state is a linear strain-time curve.

For an applied stress of 6.23 MPa and $A_w/A_s = 1000$, Fig. 1 presents predictions of the steady-state composite creep rate relative to that of the monolithic strong phase ($\dot{\epsilon}_c/\dot{\epsilon}_s$) as a function of the volume fraction of the weak phase, V_w . Results for both strong- and weak-phase matrices are presented. Similar behavior was observed for other applied stresses and A_w/A_s ratios. Except where noted, Fig. 1 gives FEM results for the short fiber composites. Clearly, the simple analytical model accurately reproduces the FEM results for the fiber geometry. Thus, within the approximations of continuum behavior, perfect interfacial bonding, and steady-state creep in both phases, the analytical strain-compatibility model appears to be valid for this reinforcement geometry.

For the short fiber composites, Fig. 1 also shows that the predicted composite creep rate depends only on the relative amounts of the two phases, not on which is the matrix and which is the discontinuous reinforcement. Examination of the FEM results for V_w near 50% shows that switching the weak phase from the fiber to the matrix does not significantly affect the composite strain rate. This finding is not unexpected based on the success of the analytical model in reproducing the FEM results for short fibers; for a reinforcement volume fraction of 50%, the analytical model must predict the same creep rate when the properties of the two phases are interchanged.

The behavior predicted by the FEM model for spherical reinforcements is more complex than for the short fibers. For composites in which the strong phase is the matrix ($V_w < 50\%$ in Fig. 1) the creep rates are nearly the same as those predicted analytically and by FEM for short fiber composites. The similarity in creep rate for strong-matrix composites with varying reinforcement geometries also was predicted by Biner [4]. In contrast to the strong-matrix composites, Fig. 1 shows that the reinforcement shape significantly affects the deformation behavior of weak-matrix composites, just as for elastically reinforced MMCs [6,7,12,13]. For example, the creep rate for the spherical reinforcement geometry with $V_w = 78.4\%$ is almost four times greater than that of the corresponding short fiber geometry. Also note the large deviation between the analytical and FEM results for the spherical geometry. In fact, for $V_w = 78.4\%$ the creep rate predicted by FEM approaches that computed using a simple iso-stress rule-of-mixtures model. FEM calculations show that the high creep rate for the spherical geometry is due to a less effective transfer of stress from the weak matrix to the strong reinforcement compared with the fiber geometry [14].

As stated in the Introduction, one goal of this study was to determine the effect of a creep-weak phase on the creep rate of a strong matrix material. Focusing on the short fiber geometry, Fig. 2 presents FEM predictions of the relative composite creep rate as a function of

Figure 1. FEM and analytical predictions of the relative composite creep rate as a function of the volume fraction of weak phase, V_w , for $A_w/A_s = 1000$.

Figure 2. The effect of A_w/A_s ratio on the relative composite strain rate predicted by FEM for short fiber composites with a strong matrix and $n_w = n_s = 4.9$.

the disparity in monolithic creep rates, *i.e.* A_w/A_s , for two weak fiber volume fractions. In addition, an upper bound on the composite creep rate was computed by replacing the fiber with a void, thereby reducing the net section of material available to carry load. The FEM results of this "loss-of-section" model are indicated in Fig. 2 for the two fiber fractions. Figure 2 shows that the composite creep rate increases as A_w/A_s increases, apparently reaching the loss-of-section bound asymptotically. In general, for the case of $n_w = n_s = n$, the creep resistance of the strong phase tends to be less severely degraded by the weak phase if V_w , A_w/A_s , and n are small. For example, for $n = 4.9$, Fig. 2 shows that the relative composite creep rate, $(\dot{\epsilon}_c/\dot{\epsilon}_s)$, is less than 10 if $V_w = 21.6\%$ or if $V_w = 51.2\%$ and $A_w/A_s < 500$. Relative creep rates above 10 are predicted for $V_w = 51.2\%$ and $A_w/A_s > 500$. Similar calculations using $V_w = 51.2\%$ but setting $n = 1$ predict that the relative composite creep rate saturates at a value of only about 2 for $A_w/A_s \geq 1000$. For $n = 10$, however, the same calculations show a relative composite creep rate of about 75 when $A_w/A_s = 10^5$, compared with a value of only 23 for $n = 4.9$ (Fig. 2).

The iso-strain analytical model successfully predicts the steady-state composite creep rate in most cases, particularly when the matrix is the strong phase (Fig. 1). However, it cannot provide details of the non-uniform internal stresses, *e.g.* the hydrostatic component, nor the localization of creep strain. Such information is valuable since it provides insights into damage accumulation during creep [6,12,13]. This provides justification for the use of FEM models, which provide the detailed field quantities, in studying these steady-state problems. As discussed elsewhere [14], the reinforcement shape significantly affects the detailed internal stress and strain states, even in cases where it has little influence on the steady-state composite creep rate. For the case of strong fibers in a weak matrix, large creep strains and hydrostatic stresses accumulate near the fiber ends, which has been associated with damage accumulation in the matrix at these locations [6,12,13]. For strong matrix, *i.e.* DPT, composites, the gradients in stress and strain appear to be somewhat less than in corresponding weak-matrix composites.

While the analytical model appears to be accurate for steady-state creep in most cases, preliminary calculations for the model composites show that it may be less accurate for transient creep. Figure 3 shows the results of calculations for a strong-matrix fiber composite in which $m_m = 0.25$. First, both models require time step sizes much smaller than those used in the steady-state calculations in order to reach a solution that is essentially independent of time step size. The difficulty in converging on an accurate solution appears to be due to the continuous redistribution of stresses within the composite during transient creep. Second, there is a clear

(3)

(4)

Figure 3. Analytical and FEM predictions of the creep curve for a model composite in which the matrix material exhibits primary creep.

Figure 4. Predictions of the steady-state creep rate as a function of the applied stress are compared with data for Nb-Si alloys. Data of Subramanian *et al.* [5].

deviation in the creep curves predicted by the two models. For a time of 2000 s, there is a 14.4% difference in the predicted creep strains. Preliminary analysis suggests that this discrepancy results from the better representation of the internal stresses and their redistribution using FEM compared with the simple analytical model.

It is desirable to compare the predictions of the models described here with data for real DPT IMCs. To do so, creep data are required for the composite and its component phases. Unfortunately, such data sets are scarce. However, comparison of the model predictions can be made using the preliminary data of Subramanian *et al.* [5] for a Nb₅Si₃/Nb in-situ composite. This composite was produced by casting a Nb-10%Si alloy, extruding to a 10:1 ratio at 1482 °C, and annealing at 1500 °C for 100 h. The resulting composite had a complex microstructure consisting of approximately 73% Nb-Si solid solution phase in a matrix of the intermetallic. Based on the strong matrix results in Fig. 1, it was assumed that the exact phase morphology does not significantly affect the composite creep rate, so this material was modeled as a regular array of ductile fibers in a matrix of Nb₅Si₃.

Figure 4 presents the salient data gathered by Subramanian *et al.* at 1200 °C. The steady-state creep properties of the intermetallic were computed from the data in Fig. 4, giving: $n_m = 1.0$, $A_m = 3.63 \times 10^{-11} \text{ (MPa} \cdot \text{s)}^{-1}$. For the ductile solid solution, the creep properties were estimated from those of the Nb-4%Si alloy data shown in the figure, giving: $n_f = 4.68$, $A_f = 2.98 \times 10^{-16} \text{ (MPa}^{4.68} \cdot \text{s)}^{-1}$. Using these values, the circles in Fig. 4 show the predicted steady-state creep rate of the composite. Both models predict the same results, as expected for this strong matrix composite (see Fig. 1). The predicted composite stress exponent is approximately 1.0, as expected from the results of model system calculations showing that the composite stress exponent essentially equals that of the slower creeping phase, in this case Nb₅Si₃. Unfortunately, the preliminary data do not allow for confirmation of this prediction. However, comparison of the absolute creep rate for the Nb-10% Si composite with the predicted rate is possible for an applied stress of 100 MPa. At this stress, the predicted creep rate is more than an order of magnitude less than the experimental value. A similar creep rate was predicted using pure Nb as the ductile phase, which creeps much faster than Nb-4%Si. Based on the earlier discussion of Fig. 2 and the fact that $n = 1$ for the intermetallic, the insensitivity of the predicted composite creep rate to the ductile phase properties is not unexpected. One possible reason for the discrepancy between the experimental and predicted creep rates is that microcracks and voids were observed following creep testing of the composite. These damage processes are not

included in the models, contributing to a predicted creep lower than the experimentally observed value.

CONCLUSIONS

Based on analytical and finite element method continuum analyses of deformation in composites for which both phases exhibit creep, the following conclusions have been drawn.

1. For strong matrix IMCs, the simple analytical model based on strain compatibility between phases predicts composite creep rates consistent with those computed by the finite element method. However, significant deviations in the strain vs. time curves predicted by the two models occur for transient creep.
2. The steady-state composite creep rate is predicted to be nearly independent of the reinforcement geometry for ductile-phase toughened composites, for which the matrix is the strong phase.
3. For ductile-phase toughened IMCs, the addition of the weak ductile phase is predicted to degrade the creep resistance of the intermetallic more severely with increases in the stress exponent of the intermetallic and the volume fraction and creep rate of the ductile phase.
4. Unlike simple analytical models, the finite element method provides detailed internal stress and strain distributions that can provide insights into possible damage accumulation during creep.
5. Predictions of the steady-state creep rate for a Nb₅Si₃/Nb in-situ composite deviate from the data by more than an order of magnitude. This discrepancy may be due in part to the evolution of damage observed in composite, which is not treated in the models.

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