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Simulation of Fatigue Behavior of High Temperature Metal Matrix Composites

ABSTRACT: A generalized relatively new approach is described for the computational simulation of fatigue behavior of high temperature metal matrix composites (HT-MMCs). This theory is embedded in a specialty-purpose computer code. The effectiveness of the computer code to predict the fatigue behavior of HT-MMCs is demonstrated by applying it to a silicon-fiber/titanium-matrix HT-MMC. Comparative results are shown for mechanical fatigue, thermal fatigue, thermomechanical (in-phase and out-of-phase) fatigue, as well as the effects of oxidizing environments on fatigue life. These results show that the new approach reproduces available experimental data remarkably well.

In today's globally competitive environment, structural systems need not only perform satisfactorily and reliably, but must also be cost-effective. One of the key questions in highlighting a new structural system is "what material will provide the optimum combination of performance and cost?" The majority of the cost component is usually the cost of extensive test data used to characterize the material, not the material cost. The most often asked question, "how many test data do we need to characterize the material?" should be changed to "how can be quantify the materials behavior with minimum test data?" That is, there is a need to presume and quantify the constituent materials behavior that should be done via computational simulation and by taking advantage of high-speed computer platforms.

As the understanding of different materials and the numerous variables that affect them grows, many different material and service-environment specific models are developed [1]. For instance, different models are used for different metallic-matrix composite materials under different in-service static, dynamic, creep, and fatigue loads [2]. Despite the sophistication of these models, they usually constitute data fitting to various degrees of success. Further, they are not inclusive of (1) predominant factors contributing to coupled nonlinear material behavior; (2) all material thermal, mechanical, and other relevant properties; and (3) the entire material history from fabrication to sustained load use and to fracture. To

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understand these specific and limited-in-scope models, investigators have traditionally relied on test data. Clearly, there is a need for one single material characterization model that can quantify all of the requisite effects, starting from primitive variables at the lowest constituent material scale for the whole composite life, with a minimum need for test data.

NASA Lewis Research Center has been, for more than two decades, pursuing alternative general-purpose theories for quantifying coupled nonlinear material behavior [3–5]. This approach is based on computational simulation of the entire physical process that governs the coupled material behavior [6,7]. The objective of the present investigation is to describe the application of the theory for computationally simulating the thermomechanical cyclic behavior of high temperature metal matrix composites (HT-MMCs) via a single model. The computer code that evolved to perform the computational simulation is described briefly in this paper, with suitable references for more details. The authors hope that the reader will focus on why and what can be done, and will rely on the references for the subtleties on how.

Computational Simulation of Fatigue

In this section, we describe the fundamentals underlying the computational simulation approach along with its respective computer codes. Then, we proceed to describe its effectiveness to simulate mechanical fatigue, thermal fatigue, thermomechanical fatigue, and oxidative effects.

Fundamental Considerations

The computational simulation of HT-MMCs, as described herein, is based on (1) what constituents the composite materials are made from; (2) how their material behavior is manifested at their progressively interactive multiple scales, including the effects of how they are made; (3) how the composite structures respond to service environments; (4) what governs their behavior under a desirable set of design requirements; (5) how the solution of the fundamental governing field equations for all the participating variables is obtained by employing the computer as an integral part of the solution; and (6) how the evolution of the behavior or process is simulated.

By using this simulation, we are able to model various types of effects on the materials behavior such as: (1) service loads, mechanical and thermal; (2) cyclic effects; (3) time effects including creep; (4) temperature effects; (5) chemical and metallurgical effects, such as oxidation; and (6) fabrication-induced stresses.

The simulation starts with constituents and the fabrication-process, and proceeds to unfold the effects induced by the aggressive service loading environments at the structure scale. The structure scale response for a load increment, along with incremental environmental effects, are then used to update the materials behavior at the constituent scale, thus accounting for all the mutual interaction effects. These effects are synthesized up to the structure scale to obtain an up-dated structure deformed position, and the process is repeated until an equilibrium position for the structure is obtained. Next, the loads and environments are updated to their next increments, and the cycle is repeated until the onset of structural fracture is reached. This process is described for a specialty computer code in the next section.

METCAN Computer Code

The METAL matrix Composite Analyzer, METCAN, computationally simulates the materials behavior of HT-MMCs from micromechanics to laminate [8]. The structure of METCAN parallels the fabrication process of HT-MMCs. The schematics in Fig. 1 illustrate
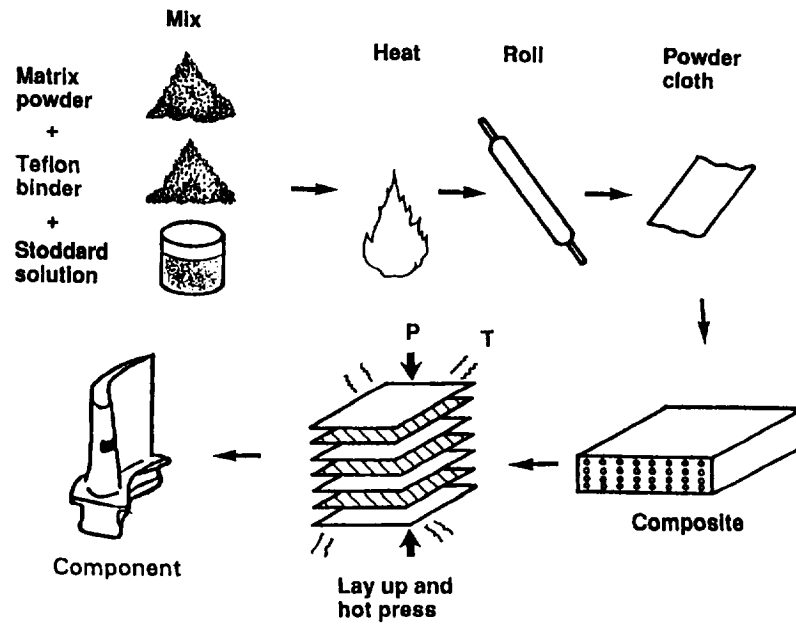
FIG. 1—*Metal-matrix composite fabrication process.*

a typical fabrication process. Figure 2 shows the computational sequence for the simulation of composite behavior including the fabrication process. The sequence consists of: Step I—processing, cool down from processing temperature to room temperature; Step II—heat up to use temperature from room temperature; and Step III—mechanical load to obtain stress-strain data. METCAN is capable of predicting the entire HT-MMC behavior history, including the fabrication process by using only room temperature properties for the fiber, matrix, and interphase.

The METCAN simulation capability is shown in Fig. 3. The simulation starts from describing the material properties at the constituent (fiber/matrix/interphase) scale and synthesizes the ply and laminate scale properties through composite micromechanics, macromechanics, and laminate theories (left-hand side of Fig. 3). The laminate scale
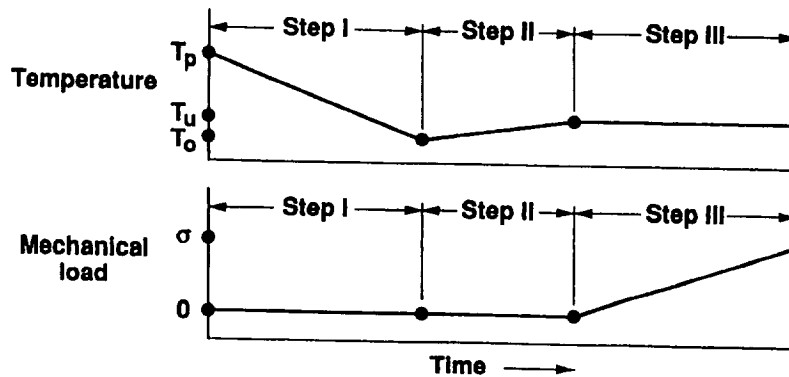

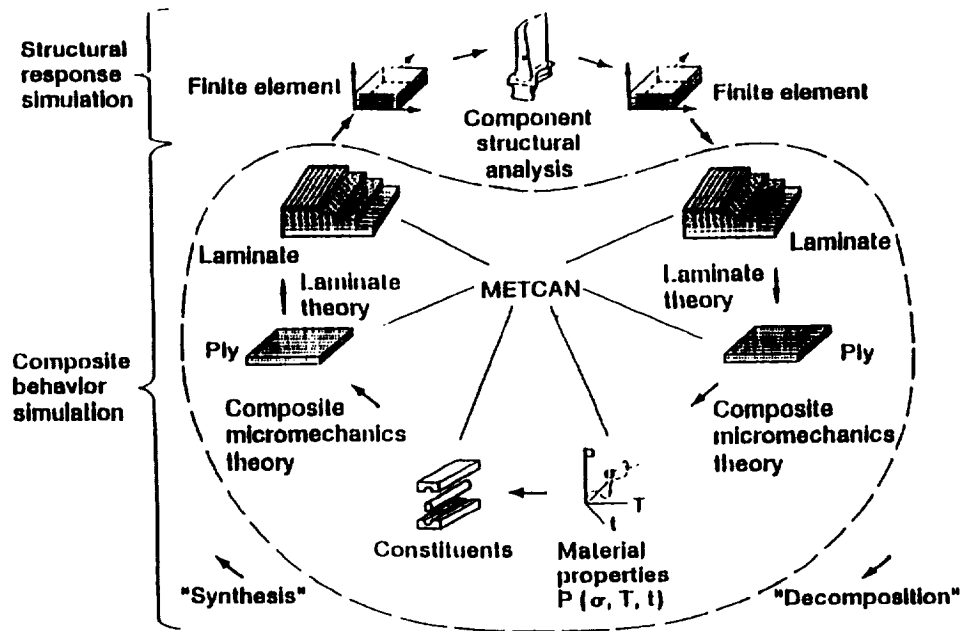FIG. 2—*METCAN computational simulation sequence.*

FIG. 3—*METCAN computational simulation of high temperature intermetallic matrix composite behavior.*

properties are used for the global structural analysis (top of Fig. 3). The global structural response is then decomposed to the laminate, ply, and constituent scales (right-hand side of Fig. 3). A detailed description of the micromechanics used for representing the simulation at the constituent materials scale is given in Ref 7. The room temperature properties of the lowest scale constituent materials are automatically extracted from the METCAN resident data bank that can be augmented for properties of new materials. The data bank is designed to include all room temperature thermal, mechanical, and oxidative properties and their respective exponents for dependence on all types of variables such as temperature, time, and stress. This feature results in a considerable saving of time required for searching and inputting the composite material property data.

Multi-Factor Interaction Model

We start with the premise that if we are to capture all the variables that affect the materials behavior, we need a unified description. Figure 4 shows an n-dimensional material behavior space (MBS) where each dimension represents a specific aspect of material behavior. It is reasonable to assume that the MBS can be described by an assumed interpolation function. One convenient function is a polynomial of product form because mutual interactions can be represented by the overall product to include cross products that are common in higher-degree algebraic polynomials. In this context, the MBS is assumed to be described by a multi-factor interaction model (MFIM) as follows
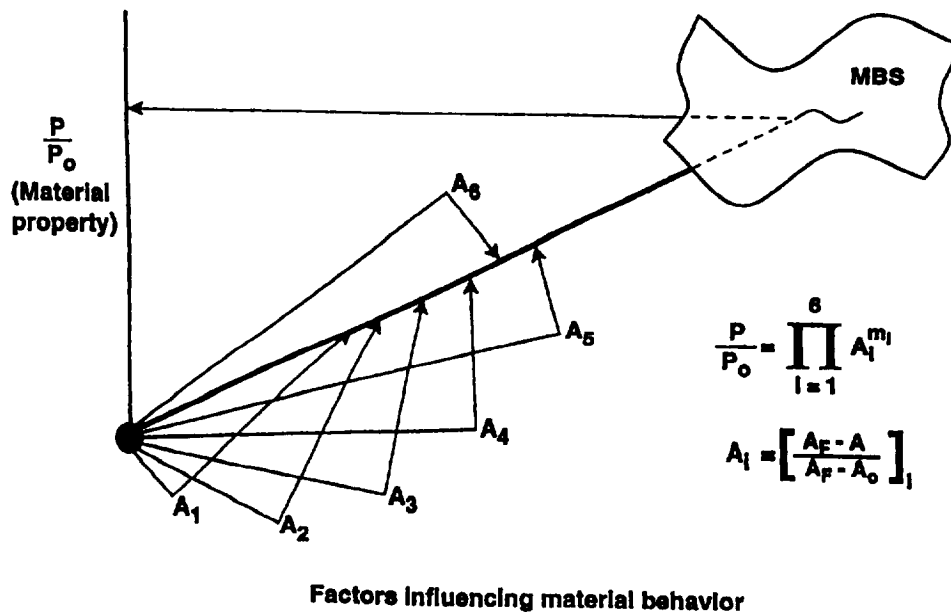
$$\frac{P}{P_0} = \prod_{i=1}^{n} A_i^{m_i}$$

(1)

Factors influencing material behavior

FIG. 4—*Multi-factor interaction model for material behavior space (MBS).*

where P is any material property at current conditions. A_i represents the ith factor that influences the material behavior, m_i denotes the material exponent, and n is the number of factors that affect the material behavior in that specific application. The subscript, 0, refers to the reference condition. The exponent, m_i, is selected from known material behavior. For new materials, m_i can be determined from a few selected tests or from the "best judgment" of a materials expert [9]. The form of the factor, A_i, is taken to be
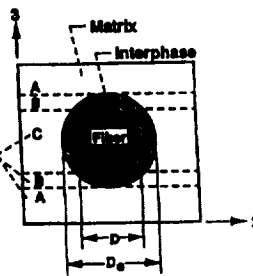
$$A_i = \left(\frac{A_i - A}{A_i - A_0} \right)_i \tag{2}$$

The subscripts, 0 and F, refer to the reference and final (or future) conditions, respectively.

Representing the MBS by the MFIM (Eq 2) has another distinct advantage. The factors, A, themselves can also be represented by another level of MFIM or progressive substructuring of Eq 1. This progressive substructuring leads to a multi-tier representation of the MBS that permits intrinsic "lower tier" behaviors to influence more than one factor at the next higher tier. When this is done, n can be limited to a small number but the number of factors influencing the material behavior at the next lower tier will increase exponentially as n' where j is the number of that tier. For example, when $j = 1$, the number of factors (n) is 4; $j = 2$, $n = 16$; $j = 3$, $N = 64$, etc. This representation is natural for multi-parallel processing machines where the levels of tiers are programmed for different granularities. Obviously, then, the motivation for selecting such a form is for programming convenience and for computational efficiency.

The MFIM general-purpose form is amenable to unlimited extensions for describing the interactive effects of all types of physical (mechanical, thermal, metallurgical, chemical, etc.) variables in one single equation. An expanded form of the MFIM showing typical physical variables and reasons for their selection are summarized in Fig. 5. It is to be noted

$$\frac{P}{P_0} = \left[\frac{T_F - T}{T_F - T_0}\right]^l \left[\frac{S_F - \sigma}{S_F - \sigma_0}\right]^i \left[\frac{S_F - \sigma}{S_F - \sigma_0}\right]^m \left[\frac{T_F - \sigma}{T_F - \sigma_0}\right]^n \left[\frac{R_F - R}{R_F - R_0}\right]^p \cdots$$

$$\cdots \left[1 - \frac{\sigma_M N_M}{S_F N_{MF}}\right]^r \left[1 - \frac{\sigma_T N_T}{S_F N_{TF}}\right]^s \left[1 - \frac{\sigma_t}{S_F t_F}\right]^u \cdots$$

Subregions of
intralaminar
nonuniformity

Rationale:

- Gradual effects during most range, rapidly degrading near final stages
- Representative of the in situ behavior for fiber, matrix, interphase, coating
- Introduction of primitive variables (PV)
- Consistent in situ representation of all constituent properties in terms of PV
- Room–temperature values for reference properties
- Continuous interphase growth
- Simultaneous interaction of all primitive variables
- Adaptability to new materials
- Amenable to verification inclusive of all properties
- Readily adaptable to incremental computational simulation

Notations:

P – property; T – temperature; S – strength; R – metallurgical reaction; N – number of cycles;
t – time; over dot – rate; subscripts: O – reference; F – final; M – mechanical; T – thermal

FIG. 5—*Assumed multi-factor interaction model (MFM) to represent the various factors that influence in situ constituent materials behavior.*

that the exponents in the MFIM represent monotonic shape or the path of the material behavior. For example $-\infty <$ exponent $< \infty$ covers the whole MBS. Obviously, MFIM is amenable to simulating rates-of-change of materials behavior. The inclusiveness of this particular form combined with its simplicity make it very effective for computational simulation. Note that effects not present in the specific application are represented by using "zero" exponent for the respective terms in MFIM. Complete bond was assumed for the simulation described herein. Partial bond is accounted for by voids or low-moduli at the interfaces.

Mechanical Fatigue

In this section, we describe the application of METCAN to predict the mechanical (mechanical load cyclic stress) fatigue for HT-MMCs. Two isothermal cases are described: mechanical fatigue at room temperature and mechanical fatigue at high temperature.

Room Temperature—METCAN simulation results are shown in Fig. 6 where limited data [9] are also shown for comparison. The constituent material properties for these comparisons are listed in Table 1. METCAN simulation results reproduce the experimental data (static and cyclic) remarkably well. METCAN simulations for microstresses also help to identify regions of predominant failure mechanisms as is illustrated in Fig. 6. The information in Fig. 6 can be used to assist characterization of fracture surfaces obtained from fractographic studies.

High Temperature—METCAN simulation for this case is shown in Fig. 7 where, for three different frequencies, data [9–11] are also shown for comparison purposes. The simulation results follow the test data reasonably well. The authors consider these comparisons remarkable, since the simulation uses only room temperature data for the constituent material properties and an average fiber volume ratio of 0.35, while the data ranged from 0.3 to 0.45. The agreement can be improved by selecting the exponents appropriately for each different material (calibration) [12]. The simulation is based on micromechanics and in-
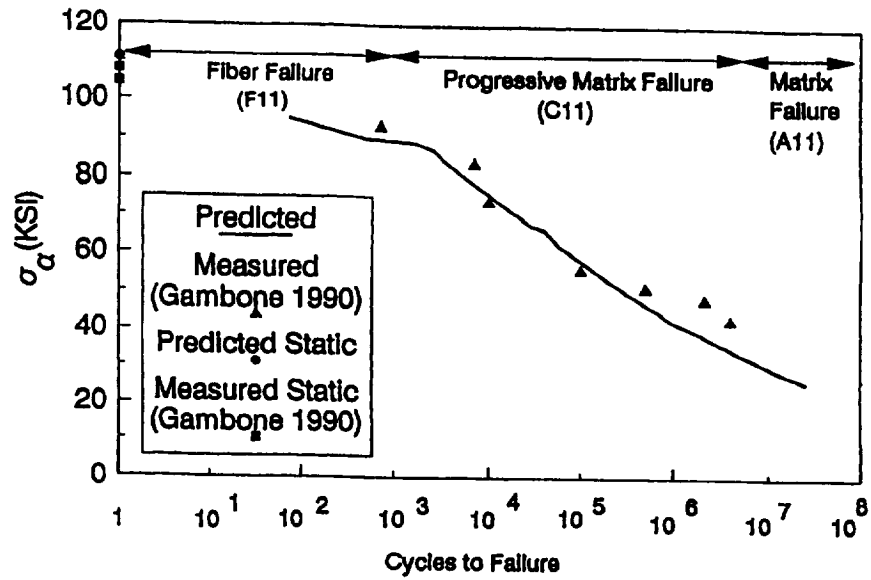
FIG. 6—*Predicted isothermal fatigue life (23°C, R = 0.1).*

TABLE 1—*Constituent (fiber/matrix) material properties used in METCAN.*

|	Material Properties			
	Fiber		Matrix	
	SiC	SiC	Ti-15-3	Ti-6-4
ρ, lb/in.^{3}	0.110	0.108	0.172	0.170
T_m, °F	4870	4500	3000	3000
E_{11}, Mpsi	62	60	12	17
E_{22}, Mpsi	62	60	12	17
G_{12}, Mpsi	26	20	5	7
ν_{12}	0.19	0.30	0.32	0.30
α_{11}, ppm/°F	2.7	2.7	4.7	5.2
α_{22}, ppm/°F	2.7	2.7	4.7	5.2
S_{11}, ksi	500	500	60	74
S_{22}, ksi	500	500	60	74
S_{12}, ksi	300	250	36	44
ρ^{gm}/cm^3	3.06	3.0	4.8	4.72
T_m (°C)	2688	2482	1649	1649
E_{11} (Gpa)	427	414	82.7	117
E_{22} (Gpa)	427	414	82.7	117
G_{12} (Gpa)	179.3	138	34.5	48.3
ν_{12}	0.19	0.30	0.32	0.3
α_{11} (ppm/°C)	4.9	4.9	8.5	9.4
α_{22} (ppm/°C)	4.9	4.9	8.5	9.4
S_{11} (Gpa)	3.5	3.5	0.413	0.51
S_{22} (Gpa)	3.5	3.5	0.413	0.51
S_{12} (Gpa)	2.07	1.7	0.25	0.3
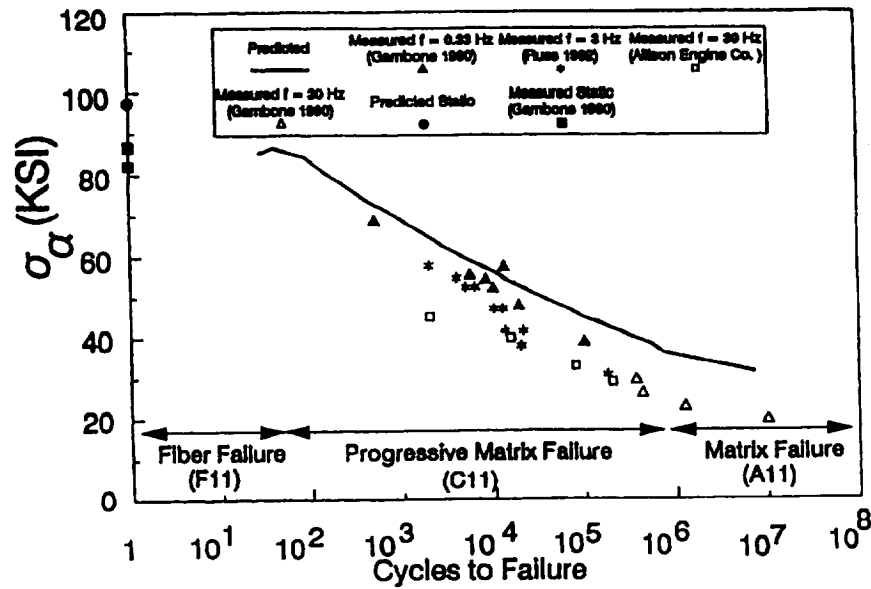
FIG. 7—*Predicted isothermal fatigue life (650°C, R = 0.1).*

cludes the fabrication process effects and all nonlinear effects through the MFIM. We can confidently conclude that the METCAN simulations are credible.

Note that F11, C11, and A11 in Figs. 6 and 7 refer to the fiber and matrix regions as depicted in Fig. 5.

Thermal Fatigue

METCAN has successfully been used to simulate thermal fatigue. Typical results from such simulations together with limited experimental data [12] are shown in Fig. 8. The constituent material properties for these simulations are listed in Table 1. METCAN predicted the composite properties that are compared with measured data in Ref 12. The simulation was performed by cycling the specimen at the thermal stress in the N_T term in the MFIM (Fig. 5) and then loading it to fracture in tension as depicted in the schematics in Fig. 8. It can be seen in Fig. 8 that the comparisons are in excellent agreement.

This excellent agreement demonstrates that the mechanics embedded in METCAN effectively represent the physics of HT-MMC behavior at all its inherent scales and throughout the load history from the fabrication process to fatigue life at elevated temperatures. Additionally, these comparisons also demonstrate the inclusiveness of the MFIM to describe the various effects on the constituent materials behavior.

Thermomechanical Fatigue

The application of METCAN to computationally simulate thermomechanical fatigue (TMF) is described in this section. Both types of TMF, in-phase and out-of-phase, are simulated. Their respective history sequence is shown in Fig. 9.

METCAN simulation results for 0.35 fiber volume are shown in Fig. 10 for both TMF lives in non-oxidizing environments where limited data [13] are also shown. As can be seen,
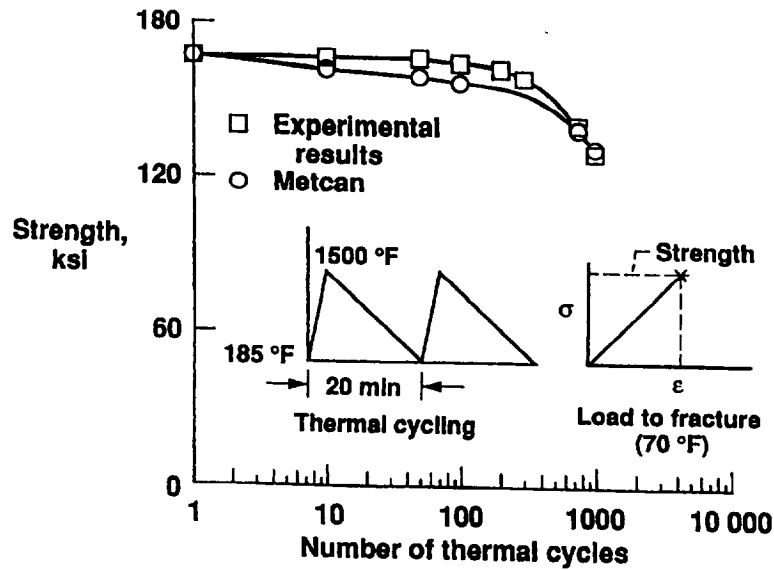
FIG. 8—*METCAN simulated thermal fatigue degradation effects of unidirectional SiC/Ti composite at fiber volume ratio (FVR) 0.36.*
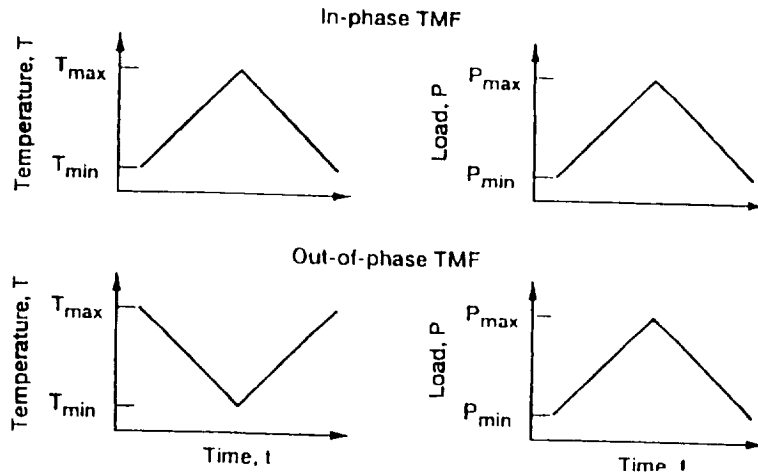

FIG. 9—*In-phase and out-of-phase TMF loading history.*

METCAN simulates the data remarkably well. The oxidizing environment included the N_{xf} and N_f terms in the MFIM in Fig. 5.

Corresponding results for the TMF lives in oxidizing environments are shown in Fig. 11. Here, again, METCAN simulates the data remarkably well. The oxidation effects on TMF were obtained by activating the (R) term in the MFIM in Fig. 5 as was already mentioned.

METCAN simulation results for the same composite but for a different thermal cycle range are shown in Fig. 12 where limited data [13] are also shown for comparison purposes. The comparisons between the two are remarkably close, demonstrating the simulation
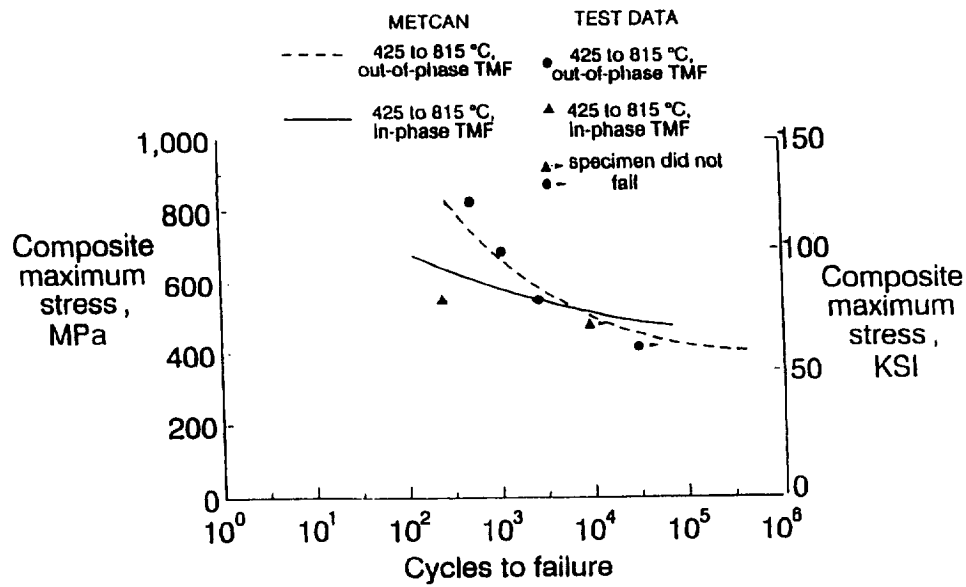
FIG. 10—*TMF lives of [0°] SiC/Ti-24Al-11Nb in flowing argon.*
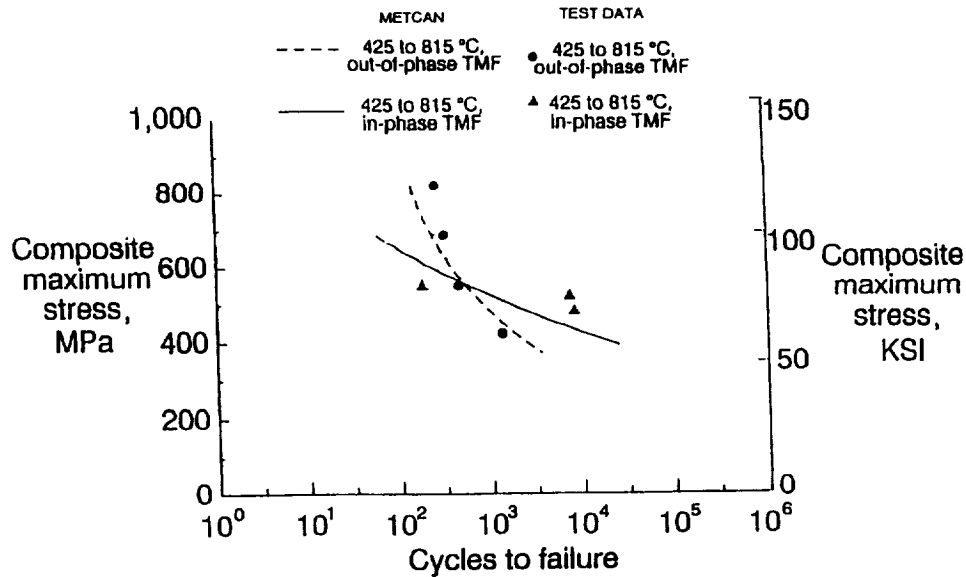
FIG. 11—*TMF lives of [0°] SiC/Ti-24Al-11Nb in air environment.*

versatility of METCAN for oxidizing effects, time dependence, and temperature dependence. It is important to note that the combined cyclic and oxidizing environment degrade the material as predicted by the MFIM. Failure is determined by loading the specimen to fracture in that mode. The local failures are determined by comparing the local micro stress component with its respective uniaxial strength at that region.
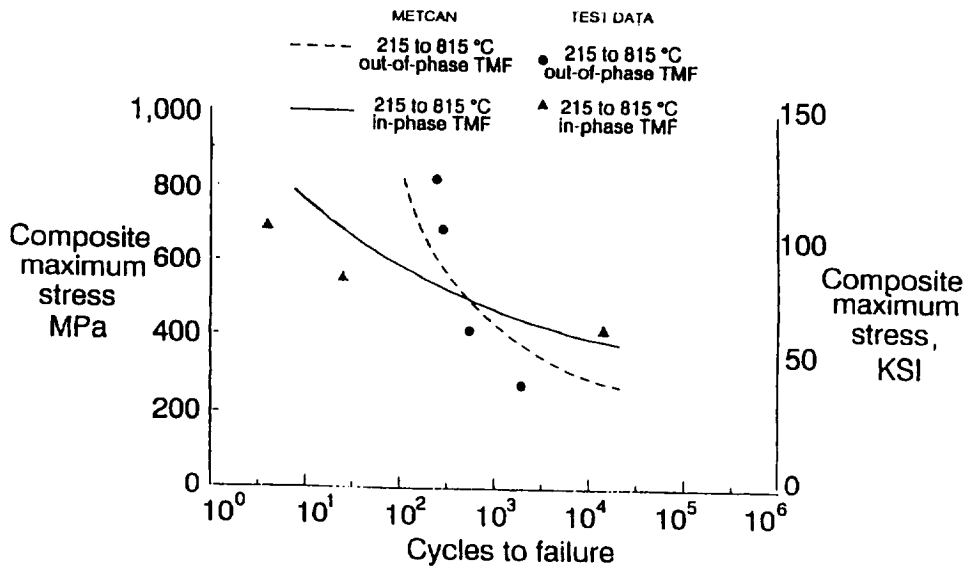
FIG. 12—*TMF lives of [0°] SiC/Ti-24Al-11Nb in air environment.*

General Comments

The previous discussion addressed METCAN simulation of HT-MMC fatigue behavior. Fatigue life is a very important aspect of these composites and, in addition, it serves as a direct means to demonstrate the effectiveness of METCAN simulation, in general. The simulation generality lies in the mathematical expressions (equations) that are used to describe HT-MMC mechanics [14]. The effectiveness of METCAN to simulate hot composite structures made from HT-MMCs has also been demonstrated [15]. Furthermore, METCAN's effectiveness for static monotonic progressive fracture has been demonstrated [16]. The discussion was limited to unidirectional composites because those were the only data we had for comparison. METCAN can handle any laminate configuration including hybrids.

It was hinted throughout the discussion that the effectiveness of the MFIM lies in having credible final values for the various factors in the expanded equation (Fig. 5). Credible final values for various factors may not be available especially for new materials or for long-term effects. The third author recommends an induction-type approach in conjunction with behavior-specific experiments to determine credible final values. The induction-type approach works as follows: (1) to predict the fatigue behavior for known conditions; (2) to simulate the fatigue behavior by extrapolating to a higher number of cycles but lower cyclic stress amplitude; (3) to perform experiments with extrapolated conditions and compare the results; and (4) if the results agree, to repeat Steps 2 and 3 until confidence has been obtained to establish credible final values.

At its present status, the authors consider METCAN a desk-top "virtual test laboratory" to rapidly evaluate the HT-MMC fatigue behavior as well as any other behavior in general. What is more important is that all the simulations are consistent because they are based on the same constituent materials, the same fabrication process, and the same model for all effects.

Conclusions

The important conclusions of this investigation to computationally simulate the fatigue behavior of high temperature metal matrix composites (HT-MMCs) are as follows:

1. Computational simulation, with its attendant computer code, is an effective and general approach to simulate the fatigue behavior of HT-MMCs.
2. The computational simulation is inclusive of the various effects (processing, cycles, stress-amplitude, temperature, oxidative environments, etc.) that affect fatigue behavior or fatigue life, or both.
3. Comparative results for mechanical, thermal, thermomechanical, and oxidative effects demonstrated that computational simulation reproduces experimental data remarkably well.
4. The computational approach, with its attendant computer code, provides a desk-top virtual test laboratory to rapidly evaluate the fatigue behavior of HT-MMCs.

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