Micromechanism Based Modeling of Structural Life in Metal Matrix Composites

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This report details the most recent accomplishments that have lead towards the fulfillment of the grant objectives. These achievements include: 1) life prediction of continuous fiber metal matrix composites; 2) the influence of heat treatment on the mechanical properties and damage development in a SiC/Ti-15-3 MMC; 3) the experimental characterization of oxidation on fracture surfaces and crack growth behavior; 4) modeling the effects of oxidation on the crack growth resistance of metals; and 5) the modeling of oxidation fronts in metals. In summary, the development of a low-cycle life prediction model that has the capability to account for the effect of surface oxidation on life of Titanium matrix MMC’s is complete. The research performed herein concluded that the life of the composite appears to be controlled by interface debonding and subsequent radial cracking. The work performed under this grant also included a program to experimentally characterize the morphology of TiO2, one of the primary stoichiometric oxides formed during oxidation of titanium, in order to develop more accurate oxide layer growth models. It has been shown that specimen geometry plays a significant role in the rate of oxide growth. The last phase of this research effort was to develop and numerically implement a mathematical model of oxidation for metals with the capability of modeling complex oxidation fronts, such as they arise in MMC’s. The oxidation of metals has been modeled by modifying the Fickian diffusion problem in order to simulate the chemical reaction (phase change) in the metal. The current model is capable of solving 1D and 2D oxidation problems in metallic domains with complex geometry.
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ABSTRACT

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This report details the most recent accomplishments that have lead towards the fulfillment of the grant objectives. These achievements include: 1) life prediction of continuous fiber metal matrix composites; 2) the influence of heat treatment on the mechanical properties and damage development in a SiC/Ti-15-3 MMC; 3) the experimental characterization of oxidation on fracture surfaces and crack growth behavior; 4) modeling the effects of oxidation on the crack growth resistance of metals; and 5) the modeling of oxidation fronts in metals.

In summary, the development of a low-cycle life prediction model that has the capability to account for the effect of surface oxidation on life of Titanium matrix MMC's is complete. The research performed herein concluded that the life of the composite appears to be controlled by interface debonding and subsequent radial cracking. These cracks appear to be driven by a combination of two factors: the development of a surface layer consisting primarily of stoichiometric TiO$_2$ which induces a dilational eigenstrain; and the embrittlement of material at the metal-oxide interface. In addition, the influence of various heat treatments on the mechanical behavior of SiC/Ti-15-3 MMC was also investigated. The study revealed that the heat treatments affected the overall composite compliance and damage accumulation. A model was also developed during this phase of the research, which successfully simulates the stress versus strain response of the composite accounting for both plastic deformation and damage.

The work performed under this grant also included a program to experimentally characterize the morphology of TiO$_2$, one of the primary stoichiometric oxides formed during oxidation of titanium, in order to develop more accurate oxide layer growth models. As part of this effort, the growth and structure of the TiO$_2$ oxide layer, monolithic samples of high purity titanium and Ti-15-5 were oxidized in air at 760°C for times ranging from 1 hour to a maximum of 168 hours. It has been shown that specimen geometry plays a significant role in the rate of oxide growth. In addition, the surface oxidation characteristics of Ti-15-3 MMC, while undergoing crack extension, was investigated. Results of the monotonic tension experiments on pre-cracked, then oxidized and then tested specimens indicate that the oxide layer thickness generally has little effect on the bulk behavior of the material. As part of this effort, numerical models were developed that are capable of simulating the effect of oxide on the crack growth resistance of metals. It is believed that such a model could be used to facilitate the study of the static and fatigue strength of fractured metal in an oxidizing environment. Two different methods of fracture mechanics modeling (i.e., the isoparametric and the crack closure method) were evaluated in order to simulate the mechanical response of a pre-cracked pre-oxidized specimen. The current model is capable of describing the effect of the stiffer oxide and the oxide layer volumetric expansion to the energy release rate. It has been found that the combination of these two oxide scale properties causes the energy release rate to decrease when a thin layer of oxide is present and to increase for a thick oxide layer.

The last phase of this research effort was to develop and numerically implement a mathematical model of oxidation for metals with the capability of modeling complex oxidation fronts, such as they arise in MMC's. The oxidation of metals has been modeled by modifying the Fickian diffusion problem in order to simulate the chemical reaction (phase change) in the metal. The current model is capable of solving 1D and 2D oxidation problems in metallic domains with complex geometry. Simulations of the oxide scale growth from the crack surfaces in a Ti-15-3 specimen with a semi-infinite crack, a complex geometry crack-tip, as well as the scale growth on cylindrical and wedge-like domain geometries have been successfully performed.
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Final Progress Report
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Status of Effort/Accomplishments/New Findings:

The objectives of this research effort were to: 1) develop a micromechanics and thermodynamics based model for predicting macroscopically averaged thermomechanical constitutive behavior of continuous fiber metal matrix composites (MMC's); 2) develop and test MMC's experimentally to determine microscopic variables that are necessary to develop the micromechanics model mentioned in 1); and 3) carry out a limited experimental program for model verification. In the following subsections, key accomplishments which have lead towards the fulfillment of the aforementioned objectives, are briefly summarized.

Life Prediction of Continuous Fiber Metal Matrix Composites:

The development of a low-cycle life prediction model that has the capability to account for the effect of surface oxidation on life of Titanium matrix MMC's is complete. We have observed in our own experiments (See Fig. 1) that life is reduced by a factor of five in SCS-6/Ti-β21S tested at 650°C when the composite was tested in air rather than inert gas (Argon). The life of the composite appears to be controlled by interface debonding and subsequent radial cracking, as shown in Fig. 2. This reduction in life appears to be the result of surface cracks which develop on the specimen when tested in air, as demonstrated in the SEM photo shown in Fig. 3. These cracks appear to be driven by a combination of two factors: the development of a surface layer consisting primarily of stoichiometric TiO₂ which induces a dilatational eigenstrain; and the embrittlement of material at the metal-oxide interface. The net effect of these surface features is an overall reduction in the critical energy release rate for the system. Using these observations and assumptions, we have developed a finite element model which utilizes a representative volume element (RVE) for the laminate tested above, as shown in Fig. 4. As described in our recent papers, the mesh incorporates the surface oxide layer, as well as the dilatational eigenstrain in order to capture the life reduction mechanism. As shown in Fig. 5, for the case of monotonic loading, the model does produce a reduced stress-strain behavior for the composite due to the development of surface cracks. Figures 6 and 7 demonstrate a comparison of the predicted results for cyclically loaded unoxidized and oxidized SCS-6/Ti-β21S [0₄]₄ specimen at 650°C, respectively.

Influence of Heat Treatment on the Mechanical Properties and Damage Development in a SiC/Ti-15-3 MMC:

The purpose of this study was to investigate the influence of possible heat treatments on the mechanical behavior of SiC/Ti 15-3 MMC, as well as characterize the deformation and damage mechanisms. The effects of three heat treatment conditions on the thermomechanical response and damage development in unidirectional axial and transverse specimens were investigated. A four ply uni-directional SiC/Ti-15-3 MMC was tested in the axial and transverse direction and the damage evolution at both room temperature and at 427 °C was observed. The thermomechanical study revealed that the heat treatments effected the overall composite compliance and damage accumulation.

In addition, averaging micromechanical models were utilized to simulate the effect of matrix damage and plasticity on the mechanical response of the composite. A model based on the Mori-Tanaka method was developed and implemented which combines both plasticity and damage in an incremental formulation. Model predictions were then compared to experimental results through microstructural evaluation of matrix crack densities.
Mechanical tests show that the 450°C heat treatment creates a microstructure with a consistently high elastic modulus and high damage tolerance for all loading conditions and temperatures. Microstructural evaluation identified the primary damage modes for both the transverse and axial specimens. The axial specimens showed evidence of cracks developing perpendicular to the loading direction starting from the fiber/matrix interface (see Fig. 8). The transverse specimens showed cracks emanating from areas of poor consolidation resulting in cracks propagating in the loading direction along grain boundaries. The model developed during this research initiative successfully simulates the stress versus strain response of the composite accounting for both plastic deformation and damage (see Fig. 9). In addition, a prediction of the crack density was made as a function of overall applied load. It was shown that the predicted crack density at the final load level over predicts the crack densities measured from a post-test microstructural analysis for the transverse specimens (see Fig. 10). It was believed that the over prediction was most likely due to pre-existing matrix/fiber damage.

**Experimental Characterization of Oxidation on Fracture Surfaces and Crack Growth Behavior:**

The purpose of this research was to experimentally characterize the morphology of TiO₂, one of the primary stoichiometric oxides formed during oxidation of titanium, in order to develop more accurate oxide layer growth models. In addition, this phase of the research included the preliminary design and development of a test methodology which will allow for real time evaluation of crack growth behavior in an elevated temperature (25°C to 700°C) and oxidizing (air) environment.

As part of the effort to characterize the growth and structure of the TiO₂ oxide layer, monolithic samples of high purity titanium and Ti-15-3 were oxidized in air at 700°C for time lengths as short as 1 hour to a maximum of 168 hours. Various specimen geometry’s were oxidized and then analyzed using SEM. Geometry’s investigated include: the inside radius of a small diameter hole (≤300 μm); the outside radius of a small diameter wire (≤140 μm); and a flat edge which included a corner. In addition, in order to gain insight on how the oxide layer would effect crack growth behavior and material fracture toughness, a series of experiments were conducted wherein, samples of high purity titanium were pre-cracked to a predetermined length using a fully reversed low cycle fatigue load. The crack in each specimen was wedged open and then either heat treated (in an inert environment) or oxidized at 700°C for 24 to 48 hours. Each specimen was then subjected to a monotonic tensile load where visual and tabular data were recorded for later analysis.

It has been shown that specimen geometry plays a significant role in the rate of oxide growth, as shown in Fig. 11. However, additional insight was needed in order to understand the complex strain field that appears to be present in the oxide layer during formation, as well as the predominate diffusion mechanism. Figures 12 a)-d) show typical oxide scale developed during oxidation at 700°C. The surface oxidation characteristics of Ti-15-3 MMC while undergoing crack extension is shown in Fig. 12d). The photograph indicates how oxide scale from the matrix develops around the exposed sigma fibers. Figure 13 shows how an oxide layer develops on the fracture surface during oxidation. Results of the monotonic tension experiments on pre-cracked-then oxidized-then tested specimens indicate that the oxide layer generally has little effect on the bulk behavior of the material (Fig. 14). Figure 15 a)-c) indicates that the oxide generally fractures at loads substantially below that which are required for crack growth extension of the material considered herein.
Modeling the Effects of Oxidation on the Crack Growth Resistance of Metals:

The purpose of the research was to develop a numerical model capable of simulating the effect of the oxide layer on the crack growth resistance of metals. It was envisioned that such a model would then be used to facilitate the study of the static and fatigue strength of fractured metal in an oxidizing environment.

Two different methods of fracture mechanics modeling (i.e., the isoparametric and the crack closure method) were evaluated in order to simulate the mechanical response of a pre-cracked pre-oxidized specimen. Validation of the methods is accomplished by comparing numerical results with an analytical solution for a crack in a homogeneous material (see Fig. 16), as well as crack-tip extending through a heterogeneous. Two physical characteristics of the oxide scale (i.e., the stiffness change and the volumetric expansion) were as input in the parametric numerical studies. In particular, the effect of these two parameters on the energy release rate was evaluated for a monotonically loaded, pre-cracked, compact tension specimen at room temperature.

The current model is capable of describing the effect of the stiffer oxide and the oxide layer volumetric expansion to the energy release rate. It has been found that the combination of these two oxide scale properties causes the energy release rate to decrease when a thin layer of oxide is present and to increase for a thick oxide layer, as shown in Fig. 17. An FEM model was also used to simulate a monotonic tension test on a CT style specimen that was preoxidized. Comparison to experimental results is shown in Fig. 18.

Modeling of Oxidation Fronts in Metals:

The purpose of this research was to develop and numerically implement a mathematical model of oxidation for metals with the capability of modeling complex oxidation fronts, such as they arise in MMC's.

The oxidation of metals has been modeled by modifying the Fickian diffusion problem in order to simulate the chemical reaction (phase change) in the metal. The resulting mathematical model consists of two parabolic differential equations and metal-oxide interface conditions. Two different variants of a fixed grid finite element method for numerical simulation of the oxidation process have been used. The first approach (the discrete interface method) taken was to locate the oxidation front and split the domain into metal and oxide subdomains. The second approach (the smearing front method) is based on reformulating the diffusion equations in both the oxide and metal, resulting in a single non-linear equation for the whole domain. Figures 19 and 20 show a comparison between numerical and analytical results for oxide layer thickness and oxygen concentration profiles, respectively.

The current model is capable of solving 1D and 2D oxidation problems in metallic domains with complex geometry. Validated numerical models have been used to simulate the oxide scale growth from the crack surfaces in a Ti-15-3 specimen with a semi-infinite crack (see Fig. 21), a complex geometry crack-tip (see Fig 22), in addition to scale growth on cylindrical and wedge-like domain geometries.
Personnel Supported

Faculty: D.H. Allen
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Graduate Students: J. Foulk
K.L.E. Helms
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Undergraduate: R. S. Nah
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Journal Publications


Accepted Journal Publications


Submitted

Conference Proceedings


Proceedings Volumes in Press


Book Chapters


Interactions/Transitions

a. Participation/presentations at meetings, conferences, seminars, etc.


"Oxidation and Damage in Metal Matrix Composites," Mechanics and Materials Seminar, Texas A&M University, College Station TX, February 14, 1995.


“The Effects of Oxidation and Damage on the Mechanical Response of Metal Matrix Composites,” 1995 International Mechanical Engineering Congress and Exposition, San
Francisco, CA, November 12-17, 1995.


"A Model for Predicting the Effect of Environmental Degradation on Damage Evolution in Metal Matrix Composites," ASTM Symposium on Applications of Continuum Damage Mechanics to Fatigue and Fracture, Orlando 1996.


b. Consultative and advisory functions to other laboratories and agencies, especially Air Force and other DoD laboratories.

NASA Langley
Sandia National Laboratories
Lawrence Livermore National Laboratories

c. Transitions. Describe cases where knowledge resulting from your effort is used, or will be used, in a technology application. Transitions can be to entities in the DoD, other federal agencies, or industry. Briefly list the enabling research, the laboratory or company, and an individual in that organization who made use of your research.

Provided advice on damage evolution and life in MMC's to Dale L. Ball (Lockheed-Ft. Worth, TX).

New discoveries, inventions, or patent disclosures

None

Honors/Awards

D.H. Allen, President, Society of Engineering Science
D.C. Lagoudas, Treasurer, Society of Engineering Science, IDA - DSSG member
Figure 1. Fatigue life of SCS-6/Ti-β21S [0]₄ in air and argon at 650°C.
Figure 2. Fracture surface of unoxidized SCS-6/Ti-β21S [0]₄ fatigued at 482°C for 4000 cycles.
Figure 3. Surface crack propagating radially into the interior of SCS-6/Ti-β21S [0]₄. Confirmation of embrittled layer.
Figure 4. Representative Volume Element (RVE) of the SCS-6/Ti-\(\beta\)21S [0]\(_4\) metal matrix composite. (Fiber volume fraction is 36%).
Figure 5. Comparison of elastic and viscoplastic analysis for monotonic loading of SCS-6/Ti-β21S [0]₄ at 650°C.
Figure 6. Predicted average stress vs. strain for cyclic loading of unoxidized SCS-6/Ti-β21S [0], at 650°C (first 15 cycles).
Figure 7. Predicted average stress vs. strain for cyclic loading of oxidized SCS-6/Ti-
β21S [0]₄ at 650°C (first 14 cycles).
Figure 8. Etched microstructure in transverse specimens of SiC/Ti-15-3 for each heat treatment showing dominant crack growth along grain boundary.
Figure 9. Stress vs. strain for transverse specimen of SiC/Ti-15-3 comparing simulation utilizing the crack density prediction and experimental data.
Figure 10. Prediction of crack density to applied stress for SiC/Ti-15-3.
Figure 11. Oxide layer thickness as a function of time for various geometries of Ti at 700°C.
a) Wire Ti specimen oxidized for 168 hours.

b) Flat corner of Ti-15-3 specimen oxidized for 48 hours.

c) Hole in Ti-15-3 specimen oxidized for 48 hours.

d) 4 ply SiC/Ti-15-3 CT specimen oxidized for 10 hours at 700°C.

Figure 12. Various oxidized geometries at 700°C.
Figure 13. Macro crack in Ti that has been oxidized for 24 hours.
Figure 14. Crack opening displacement as a function of load for an oxidized Ti specimen. The points a, b, and c correspond to loading conditions of 30, 50, and 70 Lb.'s respectively as shown in Fig. 15.
Figure 15. a) Fatigue crack in Ti subjected to a 30 Lb. load (point a in Fig. 14). Exposed surface (at left) and oxidized layer showing (at right).

Figure 15. b) Fatigue crack in Ti subjected to a 50 Lb. load (point b in Fig. 14). Exposed surface (at left) and oxidized layer showing (at right).

Figure 15. c) Fatigue crack in Ti subjected to a 70 Lb. load (point c in Fig. 14). Exposed surface (at left) and oxidized layer showing (at right).
Figure 16. Simplified oxide geometry for the parametric studies assumes the crack to be planer and the oxide scale to be surrounded by unoxidized metal.
Figure 17. Numerical results showing the energy release rate calculated inside the oxide layer by the isoparametric method and the crack closure method.
Figure 18. FEM model used to simulate monotonic test on an oxidized Ti CT specimen (above) and COD vs. load comparison (below).
Figure 19. Comparison of numerical and analytical results for 1D oxidation.
Figure 20. Comparison of oxygen concentration profiles along $x_2$ perpendicular to the crack surface.
Figure 21. Simulation of the location of the oxidation front in an oxidized Ti-15-3 specimen at 700°C after 0.25 hours, 0.5 hours, and 1 hour.
Figure 22. Simulation of crack tip in oxidized Ti. Actual crack tip shown above with simulation below it.