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FATIGUE IN SINGLE CRYSTAL NICKEL SUPERALLOYS
Technical Progress Report

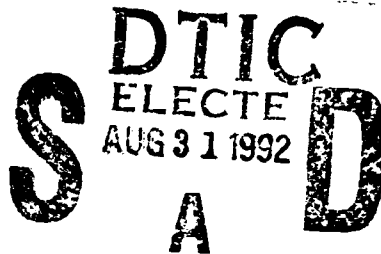
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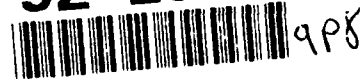


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I. Introduction and Program Objective

The fatigue initiation processes and subsequent behavior of a (single) macrocrack are fairly well documented and understood for conventional, isotropic materials. By comparison, the fatigue process in single crystal materials is significantly more complicated.

Fatigue damage in such materials is observed to involve a number of distinct 'states'. Furthermore, transition from state to state is not, as it is in more conventional materials, the simple progression of accumulated microdamage culminating in a fatigue crack of engineering dimensions. In single crystals the sequence of damage progression is greatly influenced by the regularity of the microstructure, its orientation with regard to the principal loading axis, as well as the more obvious rate-controlling parameters such as temperature, ΔK , and state of stress. The resulting macrobehavior can therefore be somewhat difficult to predict, as is evidenced by shifts in crack propagation threshold, multiplicity of cracking, and changes in crack path trajectory.

While the fatigue process is commonly described as a series of deterministic events, it is recognized that this is influenced by a stochastic component, as is any real physical process. This probabilistic influence in single crystals can be exploited to help explain the macrobehavior.

This program investigates the influence of microstructure on macrobehavior in single crystal air-foil materials by considering the micromechanics of damage accumulation as a Markov process. The program concentrates on describing mathematically this relationship with the longer term objective of establishing a model to elucidate the behavior of this complex alloy system. It is hoped that payoffs from this effort will include suggested directions for alloy improvement, as well as increased robustness against the influences of pernicious environments including hydrogen. Laboratory data is being obtained under separate funding so that this program can focus its resources on the primary objective.

To summarize, the objective of this program is to develop a micromechanistic and probabilistic model using the Markov paradigm describing the fatigue process in a class of materials which includes single crystals (i.e., the γ' strengthened superalloys).

II. Program Organization

The program is structured into three technical tasks. The individual tasks are outlined here.

Task 100 - Micromechanical Characterization

This task defines the mechanisms of damage accumulation for the various types of fracture observed in single crystal alloys. These fracture characteristics will be used to establish a series of Damage States which represent the fatigue damage process. The basis for this investigation is detailed fractographic assessment of failed laboratory specimens generated in concurrent programs. Emphasis is on specifically identifying the micromechanical damage mechanisms, relating them to a damage state, and determining the conditions required to transition to an alternate state. Principal investigator for this task is Mr. D. P. DeLuca.

Task 200 - Analytical Parameter Development

This task will extend current methods of fatigue and fracture mechanics analysis to account for microstructural complexities inherent in single crystal alloys. This will be accomplished through the development of flexible correlative parameters which can be used to evaluate the crack growth characteristics of a particular damage state. The analyses will consider the finite element and the hybrid Surface-Integral and Finite Element (SAFE) methods to describe the micromechanics of crack propagation. Principal investigators for this task are Dr. S. E. Cunningham and Mr. D. P. DeLuca

Task 300 - Probabilistic Modeling

This task will model the accumulation of fatigue damage in single crystal alloys as a Markov process. The probabilities of damage progressing between the damage states defined in Task 100 will be evaluated for input into the Markov model. The relationship between these transition probabilities and fatigue life will then be exploited to establish a model with comprehensive life predictive capabilities. Principal investigators for this task are Mr. C. G. Annis, Jr. (the Program Manager) and Mr. T. Watkins, Jr..

III. Accomplishments

One major accomplishment is an increased understanding of the micromechanics of the fatigue and fracture process in single crystal gas turbine blade superalloys. We have shown that the operative microscopic fatigue crack fracture mode can affect the fatigue crack growth rate. We have also shown that the rate of input energy (a function of stress intensity (K), stress ratio (R), and frequency (ν)) and test temperature (controlling dislocation mobility and character) determine the operative microscopic fatigue crack fracture mode.

To date we have cataloged six distinct damage states based on microscopic fatigue crack fracture modes. They are, in order of ascending energy:

1. undamaged material
2. $\gamma-\gamma'$ decohesion (submicroscopic octahedral fracture confined to the γ phase)
3. microscopic octahedral (trans-precipitate) fracture
4. ancillary decohesion (may be non-crystallographic fracture of the γ phase)¹
5. trans-precipitate non-crystallographic (monoplanar) fracture
6. trans-precipitate non-crystallographic (ancillary) fracture

These discrete states of fracture energy dissipation (separated by transition regions) are controlled by dislocation dynamics. They can possibly be modeled by Arrhenius-like rate kinetics to obtain an apparent activation energy for each discrete transition event (or end point, i.e., K_{th} and K_{IC}).

¹ This mode has been partially documented, but, as yet is not fully understood. A temperature gradient test between room temperature and 800°F is planned.

We hypothesize that these activation energies then set the energy limits between which a particular fracture mode (with its characteristic da/dN behavior) will be operative.

Markov Paradigm

- From the perspective of the Markov Paradigm these micromechanical events represent the transitional and absorbing states that determine the physical outcome of the fatigue process. The Markov model is described in greater detail in the attached ASME paper, "Markov Fatigue in Single Crystal Airfoils" by Charles Annis and Daniel P. DeLuca, presented at the International Gas Turbine and Aeroengine Congress and Exposition, Cologne, Germany June 1-4, 1992.
- We have now identified what appears to be the bulk of the microscopic fracture modes.

Significance

The identification and cataloging of these fracture states along with the correlation of fatigue crack growth (FCG) behavior represents a significant contribution to the study of fatigue and fracture and thus increased fatigue resistance through microstructural modifications based on those results. For more details on microstructural modifications which have resulted in an order of magnitude increase in LCF life in hydrogen and a 50% reduction in fatigue crack growth rate see our contract progress reports FR-21998-02 (15 December, 1991) and FR-21998-08 (15 June, 1992); also see "Improved Crack Growth in Hydrogen With Modified Precipitate Morphology Single Crystal Nickel", by D. P. DeLuca et. al., Proceedings of the Conference on Advanced Earth-to-Orbit Propulsion Technology 1992.

Planned Efforts Remaining

We will quantify Markov transition probabilities based both on statistical techniques, such as maximum likelihood parameter estimation, and through quantitative metallography identifying the relative proportion of damage in the neighborhood of the advancing crack.

We will continue to correlate fracture details with experimental FCG data currently being developed under a related program. We will also be analyzing temperature gradient FCG tests and fractures to focus on transition behavior for better resolution of these events. We will commence Task 200, Analytical Parameter Development, and continue Task 300, Probabilistic modeling.

Presentations Given and Papers Published

The paper "Markov Fatigue in Single Crystal Airfoils," by Charles Annis and Daniel P. DeLuca was presented at the International Gas Turbine and Aeroengine Congress and Exposition, Cologne, Germany June 1-4, 1992.

The paper "Improved Crack Growth in Hydrogen With Modified Precipitate Morphology Single Crystal Nickel", by D. P. DeLuca, H. B. Jones, B. A. Cowles, and F. D. Cobia was presented at the Conference on Advanced Earth-to-Orbit Propulsion Technology held at NASA George C. Marshall Space Flight Center, Huntsville, Alabama, 1992.

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Markov Fatigue in Single Crystal Airfoils

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Abstract:

This paper considers the influence of microstructure on macrobehavior in single crystal airfoils by treating the micromechanics of damage accumulation as a Markov process. Single Crystal Fatigue (SCF) is a result of several, simultaneous (competing), damage mechanisms, which are selectively favored by particular combinations of external conditions. As with any real physical process, SCF is also influenced by a stochastic component. This probabilistic influence can be exploited to help explain the macrobehavior.

We begin with a description of single crystal materials and how they differ from more conventional (isotropic) alloys. Relationships are suggested among the more probable of several competing microstructural damage mechanisms and specific rate-controlling parameters. The states of microstructural damage are then described and catalogued, and the various avenues of damage accumulation are investigated. Next, the Markov paradigm is reviewed as it applies to these materials. Finally, a Markov model is presented to describe the rather complex behavior observed in single crystals, and its use in lifing gas turbine engine airfoil is discussed.

Introduction

The difficulty of fatigue life prediction for jet engine airfoils is exacerbated by the complex behavior of single crystal materials. While the fatigue initiation processes and subsequent behavior of a (single) macrocrack are fairly well understood and documented for conventional isotropic materials, fatigue in single crystal metals is significantly more intricate.

Fatigue in such materials is observed to involve a small number of distinct states. These damage states are *not* simply numerous, successively increasing lengths of a single macrocrack, but rather microstructurally discernible conditions which comprise the damage accumulation process

itself. Furthermore, transition from state to state is not, as it is in more conventional materials, the repeated progression of accumulated microdamage culminating in an incremental advance of the fatigue crack front. In single crystals the sequence of damage progression is greatly influenced by the regularity of the microstructure, its orientation with regard to the principal loading axis, as well as the more obvious rate-controlling parameters such as temperature, loading frequency, and state of stress. The resulting macrobehavior can therefore be somewhat unexpected, as is evidenced by shifts in crack propagation threshold (Telesman and Ghosh, 1989), multiplicity of cracking, and unexpected changes in crack path trajectory (DeLuca, et al., 1991).

Characteristics of Single Crystal Materials

Modern gas turbine flight propulsion systems employ single crystal materials for turbine airfoil applications because of their superior performance in resisting creep, oxidation, and thermal mechanical fatigue (TMF). These properties have been achieved by composition and alloying, of course, but also by appropriate crystal orientation and associated anisotropy.

Early aeroengine turbine blade and vane materials were conventionally cast, equiaxed alloys, such as IN100 and Rene 80. This changed in the late 1960s with the introduction of directionally-solidified (DS) MAR-M200 + Hf airfoils. The DS process produces a $\langle 001 \rangle$ crystallographic orientation, which in superalloys exhibits excellent strain controlled fatigue resistance due to its low elastic modulus. The absence of transverse grain boundaries, a 60% reduction in longitudinal modulus compared with equiaxed grains, and its corresponding improved resistance to thermal fatigue and creep, permitted significant increases in allowable metal temperatures and blade stresses. Still further progress was achieved in the mid-1970s with the development of single crystal airfoils (Gell, et al., 1980).

The first such material, PWA 1480, has a considerably simpler composition than preceding cast nickel blade alloys because, in the absence of grain boundaries, no grain

boundary strengthening elements are required. Deleting these grain boundary strengtheners, which are also melting point depressants, increased the incipient melt temperature. This, in turn, allowed nearly complete γ' solutioning during heat treatment and thus a reduction in dendritic segregation. The absence of grain boundaries, the opportunity for full solution heat treatment, and the minimal post-heat treat dendritic segregation, result in significantly improved properties as compared with conventionally cast or directionally solidified alloys. Single crystal castings also share with DS alloys the $\langle 001 \rangle$ crystal orientation, along with the benefits of the resulting low modulus in the longitudinal direction.

Pratt & Whitney has developed numerous single crystal materials. Like most, PWA 1480 and PWA 1484 are γ' strengthened cast mono-grain nickel superalloys based on the Ni-Cr-Al system. The bulk of the microstructure consists of approximately 60% by volume of cuboidal γ' precipitates in a γ matrix. The precipitate ranges from 0.35 to 0.5 microns and is an ordered Face Centered Cubic (FCC) nickel aluminide compound. The macrostructure of these materials is characterized by parallel continuous primary dendrites spanning the casting without interruption in the direction of solidification. Secondary dendrite arms (perpendicular to solidification) define the interdendritic spacing. Solidification for both primary and secondary dendrite arms proceeds in $\langle 001 \rangle$ type crystallographic directions. Undissolved eutectic pools and associated microporosity reside throughout the interdendritic areas. These features act as microstructural discontinuities, and often exert a controlling influence on the fatigue initiation behavior of the alloy. Also, since the eutectics are structurally dissimilar from the surrounding matrix their fracture characteristics will differ.

Single Crystal Fatigue

The fatigue process in single crystal airfoil materials is a remarkably complex and interesting process. In cast single crystal nickel alloys, two basic fracture modes, crystallographic and non-crystallographic, are seen in combination. They occur in varying proportions depending upon temperature and stress state. Crystallographic orientation with respect to applied load also affects the proportion of each and influences the specific crystallographic planes and slip directions involved. Mixed mode fracture is observed under monotonic as well as cyclic conditions.

Single crystal turbine blades are cast such that the radial axis of the component is essentially coincident with the $\langle 001 \rangle$ crystallographic direction which is the direction of solidification. Crystallographic fracture is usually seen as either octahedral along multiple (111) planes or under certain circumstances as (001) cleavage along cubic planes. The fatigue and fracture processes can be visualized by relating the fractographic features to structural aspects of the alloy system. In Figure 1 the FCC unit cell structure is shown along with a depiction of the (111) crystallographic plane. Such planes in eight neighboring unit cells describe an octahedron. The fracture of an FCC specimen shown in Figure 2 displays prominent (111) octahedral shear planes.

Non-crystallographic fracture is also observed. Low temperatures favor crystallographic fracture. At higher temperatures, in the 427°C range, small amounts of non-crystallographic propagation have the appearance of transgranular fatigue in a related fine grain equiaxed alloy. Under some conditions, this propagation changes almost

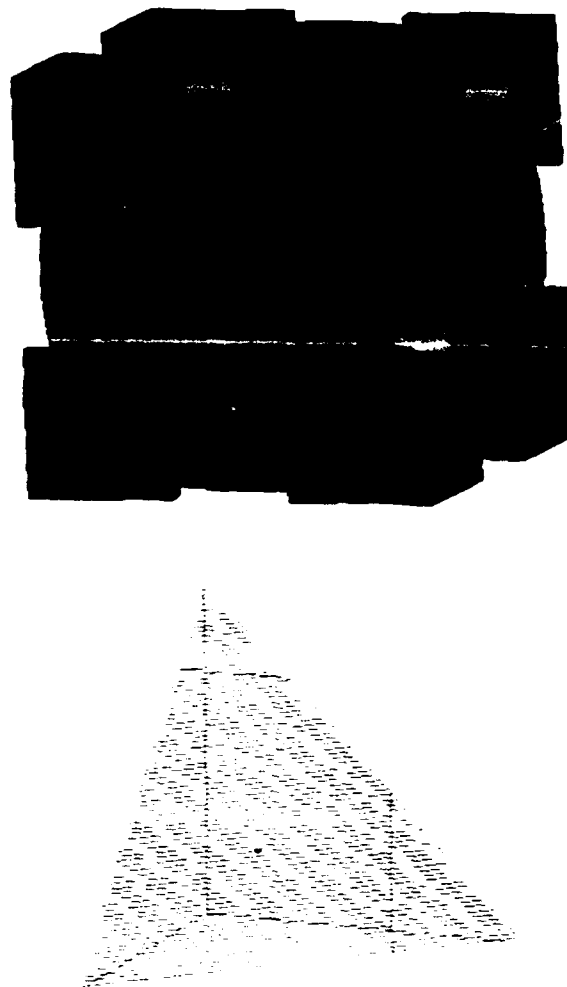


Figure 1. FCC unit cell (top) and (111) plane (bottom). Crystallographic fracture frequently occurs parallel to the (111) plane in single crystal alloys.



Figure 2. PWA 1484-HIP FCC notched specimen fracture. (1110E). Prominent (111) octahedral shear planes are visible along fatigue crack.

immediately to the highly crystallographic mode along (111) shear planes, frequently exhibiting prominent striations emanating from the fatigue origin and continuing to the final fracture region. Under other conditions the non-crystallographic behavior can continue until global failure occurs, as is seen in the turbine blade fracture surface shown in Figure 3. At intermediate temperatures (around 760C) non-crystallographic propagation is more pronounced and may continue until tensile overload, or may transition to subcritical crystallographic propagation as at 427C. At 982C propagation is almost entirely non-crystallographic, similar to transgranular propagation in a polycrystal.



Figure 3. Non-crystallographic transprecipitate fracture of a turbine blade. Such failure can occur normal to the principal loading axis at elevated temperatures and lower stresses.

Damage Catalogue

DeLuca, et al. (1991) have compiled descriptions of single crystal fracture morphologies and have postulated fatigue mechanisms for them. (This work is continuing and no claim is made that these are the only mechanisms by which single crystal materials can experience failure.) It is helpful to consider these different mechanisms as unique damage states. They are:

1. undamaged material
2. γ/γ' decohesion
3. dislocation penetration of γ' on limited (111) planes
4. local octahedral free surface formation
5. dislocation penetration of γ' on additional slip systems
6. cross slip, dislocation climb, and precipitate bypass; creep
7. global crystallographic octahedral fracture
8. non-crystallographic transprecipitate fracture

The first six of these are *transition states*, the final two are *absorbing states*. The distinction is discussed in later paragraphs.

Considerable progress has been made in understanding micromechanical cause-and-effect relationships (Dreshfield, 1986; Telesman and Ghosn, 1989; DeLuca et al., 1991). With increased understanding, however, comes the realization that many of the microstructural causes can only be determined with electron microscopy and other *ex post facto* methods. Therefore, a fatigue life prediction system requires, in addition to an understanding of the physical phenomena, a method for cataloging the relative likelihoods of these micro-occurrences, and a formalism for describing their likely interactions, the collective behavior of which constitutes the observable fatigue process. The Markov paradigm seems ideally suited to this task. Put another way, micromechanics describes the physical relationships linking damage accumulation and microstructure. But because fine microstructure is random, this information cannot be used *a priori*. Thus, a stochastic model is useful for damage prediction.

Markov Fatigue

The fatigue and fracture processes in single crystal materials can be viewed as a sequence of micromechanical events. Some of these events are transitional in that they can emerge from to enter a more damaged state; therefore, damage is accumulated in the transition from one state to another. Other states are non-transitional, or absorbing states, representing ultimate material degradation such as the creation of a thermodynamic free surface, or crack. (Since fatigue is essentially irreversible, transition probabilities from a more damaged state to one of lesser damage are defined as zero.)

Because these processes are fundamentally probabilistic in nature, the entire ensemble can be modeled as a Markov process. Here the aggregate (macroscopic) material response can be described as having resulted from sequences of microevents. While the underlying model enjoys a certain simplicity, it is remarkably powerful in describing complex, interactive behavior.

Consider an elemental volume of material being subjected to cyclic loading at some operating temperature, for example a fatigue specimen gage volume. At any given cycle count, n , (or time, or block of cycles) the damage process is in one of the states, 1, 2, 3, ... S . Let X_n represent the damage process at time n , so that the observed sequence of states is $X_1, X_2, \dots, X_n, X_{n+1}, \dots$ and so on. Under certain conditions, this sequence, or chain of events (a Markov chain) can be summarized by an $S \times S$ matrix of transition probabilities, P (equation 1).

Now let p_{ij} be the probability of transition from state i to state j . This is the conditional probability that the fatigue process will be in state $X_n = j$ at time n , given that the preceding state was $X_{n-1} = i$, that is $p_{ij} = \text{Prob}[X_n = j | X_{n-1} = i]$. If the damage process is at state i at time $n-1$, then it must be in some other (but not-necessarily different) state at time n . The

¹ The Markov assumptions here are essentially that
 (1) The future depends only upon the present, and not upon the past. Stated differently: the probabilities of future events depend only on the current state; the path which lead to that state is irrelevant. Symbolically this is

$$\text{Prob}[X_n = j | X_1 = i_1, X_2 = i_2, \dots, X_{n-1} = i_{n-1} = i] \\ = \text{Prob}[X_n = j | X_{n-1} = i].$$

 (2) These probabilities are constant over time. This provides the theoretical justification for equation 5.

movement from state i to state j is controlled by the matrix of conditional probabilities. Using 8 damage states as an example:

$$P = \begin{bmatrix} p_{11} & p_{12} & \dots & p_{18} \\ p_{21} & p_{22} & \dots & p_{28} \\ \vdots & \vdots & \ddots & \vdots \\ p_{81} & p_{82} & \dots & p_{88} \end{bmatrix} \quad \text{Eqn 1}$$

The state i is called an absorbing state if it cannot be departed once it has been entered. Thus, if i is an absorbing state, then $p_{ii} = 1$ and $p_{ij} = 0$ for all j and $j \neq i$. It is important to notice that there may be more than one absorbing state, i.e.: more than one type of failure, for example, global crystallographic octahedral fracture, or failure by non-crystallographic transprecipitate fracture.

This statistical groundwork permits answers to two main questions:

- What is the expected time, or number of accumulated cycles, required to produce failure from a given state?
- What is the probability of an early failure?

These questions can be addressed in terms of the transition probabilities. Here is a greatly simplified example.

Transition Probabilities and Fatigue Lifetimes

There is a relationship between transition probabilities and fatigue lifetime. Consider the simplest situation with only two states: state 1 is damaged, but unfractured, and state 2 is fractured. Obviously, state 2 is an absorbing state. Now p_{11} is, by definition, the probability of returning to state 1, at cycle count n , from already being in state 1 at cycle count $n - 1$. Similarly, p_{12} is the probability of becoming fractured (state 2) at cycle count n , given being unfractured (state 1) at cycle count $n - 1$. Clearly, $p_{21} = 0$ and $p_{22} = 1$. That is, the probability of becoming whole after experiencing fracture is zero, and the probability of remaining fractured is one. Notice, too, that $p_{11} + p_{12} = 1$, since if the system is currently in state 1 (the first subscript) then it must be in either state 1 or state 2 (the second subscript) at the next interval; there are no other alternatives. Thus the sum of the probabilities must be 100%. Now, if p_{11} is large (i.e. nearly one), then p_{12} is necessarily small (nearly zero), and the associated cyclic life should be longer than for a situation where, say, $p_{11} = p_{12} = 1/2$.

For this gross over-simplification, consider a sequence of events culminating in failure:

cycle: 1, 2, 3, 4, ..., $n - 1, n$
 state: 1, 1, 1, 1, ..., 1, 2

The probability of (exactly) n cycles to failure is then,

$$f(n) = p_{11} \times p_{11} \times p_{11} \times p_{11} \times \dots \times p_{11} \times p_{12} = p_{12}(1 - p_{12})^{n-1} \quad \text{Eqn 2}$$

... repeated $n-1$ times

which is the probability density of a Geometric distribution, sometimes referred to as the waiting time distribution.

For this distribution the expected, or average, cycles to failure can be shown to be $\bar{n} = 1/p_{12}$ (Mood, Graybill, and Boes, 1974). For example, if $p_{11} = 0.99$ then $p_{12} = 0.01$ and $\bar{n} = 100$. That is, if the probability of failure on any given cycle is one in one hundred, then the average cyclic life is 100 cycles to failure. If $p_{11} = 0.999$, then $p_{12} = 0.001$ and $\bar{n} = 1/0.001 = 1000$ cycles. The point is that cyclic life is a natural outcome of the state transition probabilities.

Notice, too, that the properties of the geometric distribution can be exploited to estimate the probability of an early failure, where $n < \bar{n}$. In this very simple example, the probability of a failure before N counts (or cycles) is

$$P(n < N) = \sum_{i=1}^{N-1} p(1-p)^{i-1} \quad \text{Eqn 3}$$

where p is the probability of failure on the next cycle, p_{12} in this example.

The situation is analogous for the more realistic model in which fatigue damage is catalogued into more than two damage states. The arithmetic and subsequent statistics are considerably more involved, however.

It can be shown (Taylor and Karlin, 1984) that by partitioning the transition matrix, Equation 1, into transitional and absorbing portions,

$$P = \begin{bmatrix} Q & U \\ 0 & I \end{bmatrix} \quad \text{Eqn 4}$$

with t transitional states and a absorbing states, then the $t \times t$ matrix Q is the portion of P corresponding to transitional (non-absorbing) states, and U is a $t \times a$ matrix representing the probabilities of moving from a transitional state to an absorbing state. I is an identity matrix of appropriate dimensions.

It can be further shown that

$$L = (I - Q)^{-1}U \quad \text{Eqn 5}$$

where $\mathbf{1}$ is a column matrix of ones, and L is the vector representing times to failure, from a given state.

- The expected time to failure of the undamaged material is the first element of this matrix, L_1 .

Thus the desired engineering parameter, lifetime, is obtained from the Markov description of the fatigue process.

Estimating the Model Parameters

Consider again the elements comprising the transition probability matrix in Equation 1. It is necessary that these elements be estimable for the Markov model to be a useful engineering tool. Some elements are easily determined. Because fatigue is irreversible, transitions from a more to a lesser damaged state necessarily have probability zero. Thus, all the probabilities below the matrix diagonal in Equation 1 are zero, i.e. $p_{ij} = 0$, for $i > j$. For this material there appear to be two absorbing states, global crystallographic octahedral fracture (state 7) and failure by non-crystallographic transprecipitate fracture (state 8). Thus $p_{77} = 1$ and $p_{88} = 1$ so that the lower right portion of the matrix is the 2×2 identity matrix. Now, since $p_{77} = 1$ and $p_{88} = 1$, and because the sum of the probabilities within a row must be unity, all other entries in rows 7 and 8 must be zero. Since there are six transition states and two absorbing states, the partitioned matrix is then,

$$P = \begin{pmatrix} p_{11} & p_{12} & p_{13} & p_{14} & p_{15} & p_{16} & p_{17} & p_{18} \\ 0 & p_{22} & p_{23} & p_{24} & p_{25} & p_{26} & p_{27} & p_{28} \\ 0 & 0 & p_{33} & p_{34} & p_{35} & p_{36} & p_{37} & p_{38} \\ 0 & 0 & 0 & p_{44} & p_{45} & p_{46} & p_{47} & p_{48} \\ 0 & 0 & 0 & 0 & p_{55} & p_{56} & p_{57} & p_{58} \\ 0 & 0 & 0 & 0 & 0 & p_{66} & p_{67} & p_{68} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{Eqn 6}$$

The remaining transition probabilities can be estimated from experimental observations, which include the relative proportions of crystallographic octahedral fracture and non-crystallographic transprecipitate fracture, and their average cyclic lives. The computations are conceptually straightforward but tedious in practice. The idea is to invoke the familiar least-squares criterion and select as probability estimates those values which minimize the summed squared error between these observed quantities and those predicted by the model.

Conclusions

Pratt & Whitney has enjoyed modest success in using this Markov model to explain some of the unusual behavior observed in single crystal airfoil materials in fatigue. Although only in its early development, it promises to provide a workable life prediction system for these complex materials, something which has until now proved rather elusive. The method is also being evaluated for describing damage accumulation in composite materials, again where damage is complex and does not lend itself to description in terms of a single physical entity, such as cracklength.

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