Elevated Temperature Crack Growth Rate Model for Ni-base Superalloys

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Abstract: Several time-dependent mechanisms are operational in the crack growth process of Ni-base superalloys at elevated temperature. Creep deformation during periods of sustained loading, oxygen diffusion at the crack tip, and oxidation reactions at and in front of the crack tip all contribute to the kinetics of crack growth. A crack growth rate model has been derived that attempts to capture the physics of these various rate processes. The proposed model assumes small-scale creep at the crack tip and incorporates the Hutchison-Rice-Rosengren stress field equations to satisfy this condition. The model also includes stressassisted diffusion of an environmental species at the crack tip. A process reaction rate is related to the time-rate of crack growth providing a model that accounts for these time-dependent processes. An evaluation of the form of the model is provided by comparison of the model with experimental crack growth data.

1. Introduction

Ni-base superalloys are used in a variety of high temperature applications due to their excellent creep and oxidation resistance. In applications such as turbine disks of aircraft engines these materials are subjected to elevated temperatures for sustained periods during normal operation. The typical duty cycle for a disk is modeled as a fatigue stress cycle with dwell or hold time for the purposes of predicting crack initiation and propagation life. Several timedependent damage mechanisms can operate during the cyclic loading and during the dwell period and are therefore a design and operational concern. The mechanical load and the environment can operate synergistically in a timedependent fashion to cause undesirable creep, fatigue, and oxidation damage. Along with surface oxidation, oxygen diffusion along the grain boundaries ahead of the crack tip can cause embrittlement of the material [1]. To prevent premature failure or excessive maintenance, life prediction of these components is essential. However, no comprehensive model currently exists that incorporates the various time-dependent¹ damage mechanisms. This article proposes a model that accounts for reaction kinetics, creep deformation, and oxygen diffusion during a hold period of elevated temperature operation of a Ni-base superalloy component.

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2. Environmentally-Assisted Crack Growth Rate Model Derivation

In the presence of a concentration gradient of some solute species and a potential gradient, such as a stress field, the total flux of the diffusing species is given by [2]

$$J = -D\left(\nabla C + \frac{C}{kT}\nabla U\right),\tag{1}$$

where D is the diffusion coefficient, C is the solute concentration, k is the Boltzmann's constant, T is absolute temperature, and U is the interaction potential. The continuity condition leads to

$$\frac{\partial C}{\partial t} = D\nabla \cdot \left(\nabla C + \frac{C}{kT}\nabla U\right). \tag{2}$$

The solution to Eq. (2) for the equilibrium concentration is given as [3]

$$C = C_0 \exp\left(-\frac{U}{kT}\right),\tag{3}$$

where C_0 is the concentration in the unstressed state (i.e. at the crack surface). If an elastic interaction is being considered, then [4]

$$U = p\Delta V . \tag{4}$$

When evaluating the interaction between a crack tip and a solute atom, p is the hydrostatic stress at the crack tip and ΔV is the volume change that occurs to the surrounding matrix around a solute atom. For an interstitial atom the volume change is approximated by

$$\Delta V = 4\pi\gamma^3,\tag{5}$$

where γ is the radius of the solute atom. The hydrostatic stress, p, is defined as

$$p = -\frac{1}{3} \left(\sigma_{xx} + \sigma_{yy} + \sigma_{zz} \right), \tag{6}$$

where σ_{xx} , σ_{yy} , σ_{zz} are the principal stresses in the x, y, and z directions, respectively. If Ni-base superalloys are considered, which exhibit small-scale creep during short hold times in creep-fatigue testing, then the stress field, described by the Huchison-Rice-Rosengren (HRR) equations, around a crack tip is given by [5]

$$\sigma_{ij} = \left[\frac{K^2(1-\nu^2)}{EI_n A(n+1)tr}\right]^{\frac{1}{n+1}} \hat{\sigma}_{ij}(\theta,n),$$
(7)

where K is the stress intensity factor, v is the Poisson's ratio, E is the elastic modulus, A and n are material constants for power-law creep conditions, t is time, r is the distance from the crack tip where the stress is being calculated, I_n is the HRR singular field quantity, and $\hat{\sigma}_{ij}$ represents the angular stress functions. Under plane strain conditions the hydrostatic stress can be shown to be

$$p = -\frac{1}{3} \left[\frac{K^2 (1 - v^2)}{EI_n A(n+1)tr} \right]^{\frac{1}{n+1}} [(v+1)(\hat{\sigma}_{xx}(\theta, n) + \hat{\sigma}_{yy}(\theta, n))].$$
(8)

By combining Eqs. (4), (5), and (8) and inserting into Eq. (3), the equilibrium solute concentration becomes

$$C = C_0 \exp\left(\frac{4\pi\gamma^3}{3kT} \left[\frac{K^2}{tr}\right]^{\frac{1}{n+1}} \beta\left(\hat{\sigma}_{xx}(\theta, n) + \hat{\sigma}_{yy}(\theta, n)\right)\right), \tag{9}$$

where

$$\beta = (v+1) \left[\frac{(1-v^2)}{EI_n A(n+1)} \right]^{\frac{1}{n+1}}.$$
 (10)

We can first assume that some thermally activated reaction of the solute atoms with a solvent elemental species, such as an alloying metal, is occurring. Then we can assume that the concentration of the solvent species is much greater than the concentration of the solute atoms, such that the solvent does not appreciably change with time. Also, we have to assume that the solute species is monatomic in the solvent. We then can assume a first order reaction rate for the change in concentration of the solute atoms with time and that it is given by

$$-\frac{\partial C}{\partial t} = kC, \qquad (11)$$

where the rate constant, k, is defined as

$$k = \overline{A} \exp\left(-\frac{Q}{R_G T}\right),\tag{12}$$

with \overline{A} being a constant, Q being the activation energy for the process, and R_G being the universal gas constant. Experimental evidence suggests that the crack growth rate is directly dependent on the partial pressure of oxygen for a range of pressures in and above some transitional period for some Ni-base superalloys [6]. This would be equivalent to the initial concentration of oxygen. Based on this evidence, we can make the assumption that the time rate of crack growth is proportional to the reaction rate, then

$$\frac{da}{dt} = -\alpha \frac{\partial C}{\partial t}, \qquad (13)$$

where *a* is the crack length and α is a proportionality constant. If Eqs. (9), (11), and (12) are combined and inserted into equation (13), then the crack growth rate can be written as follows

$$\frac{da}{dt} = \alpha \overline{A} \exp\left(-\frac{Q}{RT}\right) C_0 \exp\left(\frac{4\pi\gamma^3}{3kT} \left[\frac{K^2}{tr}\right]^{\frac{1}{n+1}} \beta\left(\hat{\sigma}_{xx}(\theta, n) + \hat{\sigma}_{yy}(\theta, n)\right)\right).$$
(14)

This model, then, represents the instantaneous time rate of crack growth, and it incorporates the crack tip chemical reactions, stress-assisted diffusion, time, temperature, and small-scale creep.

3. Comprehensive Crack Growth Model

A comprehensive crack growth model was developed to incorporate the thermally activated dislocation model [7] and the environmentally assisted time-dependent crack growth model. This model follows a superposition model [8]

$$\left(\frac{da}{dN}\right)_{tot} = \left(\frac{da}{dN}\right)_{cyc} + \left(\frac{da}{dN}\right)_{td}.$$
 (15)

The cycle dependent component, $(da/dN)_{cyc}$, can be divided into the athermal and the thermally activated dislocation components as follows

$$\left(\frac{da}{dN}\right)_{cyc} = \left(\frac{da}{dN}\right)_{ath} + \left(\frac{da}{dN}\right)_{dl}$$
(16)

where $(da/dN)_{ath}$ is the athermal component given by

$$\left(\frac{da}{dN}\right)_{ath} = q \Delta K^{n_1}, \qquad (17)$$

and $(da/dN)_{dl}$ is the crack growth rate component for thermally activated dislocation motion [7] which is defined as

$$\left(\frac{da}{dN}\right)_{dl} = c_0 \cdot \Delta K^{m_0 + \frac{c_1}{RT}} \cdot \exp\left(-\frac{Q_0}{R_G T}\right).$$
(18)

The time-dependent component is given by

$$\left(\frac{da}{dN}\right)_{td} = \int_{0}^{t} \frac{da}{dt} dt , \qquad (19)$$

where the time rate of crack growth is integrated over the cycle time. Also, the average crack growth rate is given by

$$\left(\frac{da}{dt}\right)_{avg} = \frac{1}{t_h} \int_0^{t_h} \frac{da}{dt} dt .$$
 (20)

Therefore,

$$\left(\frac{da}{dN}\right)_{td} = t_h \left(\frac{da}{dt}\right)_{avg}.$$
 (21)

The time rate of crack growth, which was derived in a previously is given by

$$\frac{da}{dt} = \alpha \overline{A} \exp\left(-\frac{Q}{R_G T}\right) C_0 \exp\left(\frac{4\pi\gamma^3}{3kT} \left[\frac{K^2}{tr}\right]^{\frac{1}{n+1}} \beta\left(\hat{\sigma}_{xx}(\theta, n) + \hat{\sigma}_{yy}(\theta, n)\right)\right), \quad (22)$$

which is of the form

$$\frac{da}{dt} = A' \exp\left(\Psi K^{\frac{2}{1+n}}\right),\tag{23}$$

where

$$\Psi = \Psi'\left(\frac{1}{T}\right)\left(\frac{1}{t}\right)^{\frac{1}{n+1}},\tag{24}$$

and

$$A' = A'' \exp\left(-\frac{Q}{R_G T}\right)$$
(25)

where A' and Ψ are determined from the regression analysis, Ψ' and A'' are constants, Q is the activation energy of the reaction, and t is the time at any point along the cycle. The comprehensive model can be determined by combining Eqs. (17), (18), and (20) and using the definition that $K_{max} = \Delta K/(1-R)$ to get

$$\left(\frac{da}{dN}\right)_{tot} = q\Delta K^{n_1} + c_0 \cdot \Delta K^{m_0 + \frac{c_1}{RT}} \cdot \exp\left(-\frac{Q_0}{R_G T}\right) + \int_0^{t_h} A'' \exp\left(-\frac{Q}{R_G T}\right) \exp\left(\Psi'\left(\frac{1}{T}\right)\left(\frac{1}{t}\right)^{\frac{1}{n+1}}\left(\frac{\Delta K}{1-R}\right)^{\frac{2}{n+1}}\right) dt$$
(26)

To determine the various components, the following calculation can be performed:

$$\left(\frac{da}{dN}\right)_{tot} - \left[\left(\frac{da}{dN}\right)_{ath} + \left(\frac{da}{dN}\right)_{dl}\right] = \left(\frac{da}{dN}\right)_{td}$$
(27)

The total crack growth rate, $(da/dN)_{tot}$, can be determined by obtaining a curve fit for the elevated temperature FCGR data. The $(da/dN)_{ath}$ crack growth rate can be determined from regression of room temperature data and $(da/dN)_{dl}$ is obtained from time and environment independent data acquired at elevated temperature.

The comprehensive model was determined using fatigue crack growth rate data obtained in air at 25°C and in a vacuum and in air at 704°C using 0 and 10 sec hold times for the Ni-base superalloy ME3 [7]. The following was obtained for this model through regression analysis of the data:

$$\left(\frac{da}{dN}\right)_{ath} = 7.51 x 10^{-12} \Delta K^{4.62}$$
(28)

and

$$\left.\frac{da}{dN}\right|_{tot} = 1.29 x 10^{-9} \Delta K^{3.71}$$
(29)

From regression of the vacuum test results, which should provide thermally enhanced crack growth that is independent of the environment controlled processes, the thermally activated dislocation based model was determined to be

$$\left(\frac{da}{dN}\right)_{dl} = 2.53 \times 10^{-10} \Delta K^{3.92}$$
(30)

For the thermally activated dislocation based crack growth rate model, the material constant *m* was assumed to be independent of temperature based on this same assumption being made for the ME3 data [7]. In these tests a load ratio of R = 0.1 was used. The activation energy, Q, was estimated to be the average of the activation energies calculated for the R = -0.25 (29,955 J/mol) and R = 0.50 (36,954 J/mol) data. The average value used was 33,455 J/mol.

Using the three crack growth rate results described above and assuming that the creep exponent, n, is approximately 12, which is similar to other Ni-base superalloys [9], the time-dependent crack growth rate was found to be

$$\frac{da}{dt} = 1.07x10^{-13} \exp\left(11.79K^{\frac{2}{1+n}}\right).$$
(31)

If da/dt is assumed to be constant with respect to time, Eqs. (21), (22), (23), and (24) are combined and the activation energy for the reaction of the oxygen with the alloy is assumed to be the estimated value obtained from oxidation experiments, 265 kJ/mol [7], then $(da/dN)_{td}$ can be written as

$$\left(\frac{da}{dN}\right)_{td} = 15.77t_h \exp\left(-\frac{265,000}{R_G T}\right) \exp\left(1.082x10^4 \left(\frac{1}{T}\right) \left(\frac{\Delta K}{1-R}\right)^{\frac{2}{n+1}}\right) (32)$$

The specific model that provides a first approximation for the conditions being considered for the alloy ME3 is the following

$$\left(\frac{da}{dN}\right)_{tot} = 7.51x10^{-12} \Delta K^{4.62} + 1.56x10^{-8} \Delta K^{3.92} \exp\left(-\frac{33,455}{R_G T}\right) + 15.77t_h \exp\left(-\frac{265,000}{R_G T}\right) \exp\left(1.082x10^4 \left(\frac{1}{T}\right) \left(\frac{\Delta K}{1-R}\right)^{\frac{2}{n+1}}\right)$$
(33)

Potential crack closure effects still need to be evaluated to determine if the model needs to be adjusted in some way. Regardless, agreement between the model and the experimental results as well as prediction for 5 and 30 sec hold time data is shown in Fig. 1. These results indicate a good first approximation when compared with the test data. Also, the prediction for 5 and 30 sec hold times fall within the expected locations.



Figure 1. Comprehensive model comparison with experimental results

The model shown in Eq. (33) gives a time-dependent component that is linearly proportional to hold time, and it does not fully account for the creep contribution to crack growth, since the assumption was made that da/dt was constant with time. This is true for very long times but for short times the time dependent creep component must be included. In order to compare hold times, the average time dependent crack growth rate must be determined and can be estimated by letting $t = t_h/2$. The comprehensive model is shown below. However, the constant Ψ' is not given since several different hold time tests are required to accurately determine it, as is shown in Eq. (24). This model will accurately predict the expected asymptotic behavior for long and short hold times. It incorporates the cycle and time dependent components as well as providing a means to evaluate the creep and environmental contributions.

$$\left(\frac{da}{dN}\right)_{tot} = 7.51x10^{-12} \Delta K^{4.62} + 1.56x10^{-8} \Delta K^{3.92} \exp\left(-\frac{33,455}{R_G T}\right) + 44.37t_h \exp\left(-\frac{265,000}{R_G T}\right) \exp\left(\psi'\left(\frac{1}{T}\right)\left(\frac{2}{t_h}\right)^{\frac{1}{n+1}}\left(\frac{\Delta K}{1-R}\right)^{\frac{2}{1+n}}\right)$$
(34)

4. Conclusions

The following conclusions were obtained from this analysis:

1. A model for the time rate of crack growth was derived based on stressassisted diffusion, the HRR stress field equations for small-scale creep, and oxidation reaction kinetics

- 2. A comprehensive crack growth rate model was proposed that accounted for both the cycle-dependent and time-dependent components of the fatigue crack growth rate
- 3. The proposed comprehensive crack growth rate model provided a reasonably good comparison with data obtained for the Ni-base superalloy ME3

5. Acknowledgements

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6. References

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