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Computational Viscoplasticity-Based Modeling of Stress/Strain Response in Thermomechanical Fatigue Loads

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Contemporary computing packages handle a wide variety of stress analysis types, but are yet to provide an optimal way to handle certain load cases and geometries. Blades in gas turbine propulsion systems, for instance, undergo repetitive thermal and mechanical load cycles of varied shape and phasing. Complexly-shaped airfoils create non-uniform stress paths that exacerbate the problem of FEA software attempting to determine the correct states of stress and strain at any point during the loading. This research chronicles the modernization and integration of Miller's 1976 viscoplasticity model with ANSYS finite element analysis software. Non-isothermal fatigue loadings of various types were applied to smooth specimen geometries and the results were compared to data from duplicate mechanical testing experiments. Findings indicate that this and other certain constitutive models can be integrated with software like ANSYS to handle load types that previously could not be accurately evaluated. Accurate stress-strain response via computational methods is a first step toward reliable fully-automated life prediction of parts. Such methods are powerful tools capable of helping providing safe and efficient turbine operation without the need for conservative service intervals.

Nomenclature

σ	=	applied stress
ε_{mech}	=	total mechanical strain
ε	=	nonelastic strain
R	=	rest stress
D	=	characteristic drag stress
A_1, A_2	=	material model behavioral constants
B, C_2	=	secondary calculation constants
H_1, H_2	=	hardening behavior constants
Q	=	plastic flow activation energy
n	=	loss/recovery exponent
θ'	=	temperature dependency factor

I. Introduction

EFFICIENT gas turbine operation without the need for overly conservative service intervals is of paramount importance to the energy and aerospace industries. Thermomechanical Fatigue (TMF) -capable models are a core essential in creating accurate numerical simulations that ultimately can be used as a life-prediction tool for turbine components (Ref. 1). It has been theorized that contemporary computing packages can be used to augment viscoplasticity models that display a wide range of applicability. While it is not expected that such a constitutive model could properly predict times for fracture initiation or failure, it is reasoned that predictions of approximate stress/strain states in hardening, softening, or stable regions during the lifetime of a part are quite useful. The model selected for review in this study is the 1976 Miller viscoplasticity model, which has been demonstrated to be accurate in a variety of monotonic, cyclic, high-temperature, and creep loadings (Ref. 2). The commercial computing package ANSYS was utilized to supply loadings that simulate elevated temperature low cycle fatigue

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(LCF) as well as TMF to the model. While Miller's model does not explicitly support non-isothermal cases, ANSYS can supply the model updated temperature-dependent parameters when it passes the boundary conditions with each successive simulation step (Ref. 3). Although TMF loadings can incorporate many additional sub-mechanisms and interactions not present in LCF, (Refs. 4-6) it is reasoned that simulations of the current level of sophistication can be optimized to meet an intermediary goal of providing accurate initial stress/strain responses and the associated stress histories through the first 100 cycles of a load history.

In the present study, simulation data is gathered from both Miller's unaltered model and the ANSYS augmented model under elevated LCF and TMF conditions. These results are then compared with a mixture of historical and new experimental data from matching load conditions. It is shown that the ANSYS-adapted Miller model maintains a notable degree of accuracy for simulated fully-reversed cyclic loadings in steel with significant plasticity at elevated temperatures. However, examination of the hysteresis loops and stress histories beyond the region where initial work-hardening occurs reveals increasing error versus the experimental LCF cases.
For TMF load simulations, both in-phase (IP) and out-of-phase (OP) TMF cases with similar fully-reversed strain ranges initially match the stress and strain responses of some similar experimental data well (Ref. 7). Even so, successive cycling leads to error that increases versus the experimental data earlier in the load history than in the LCF case. A mismatch or misformulation of the parameters that govern the isotropic and kinematic hardening behavior may constitute the driving mechanism behind the progressive error in both the TMF and LCF cases. The handling of the non-isothermal loads externally specifically seems to inadvertently induce an artificial kinematic hardening effect not observable in the LCF cases, as the yield surfaces can be observed to be translating with each successive cycle and increasing the peak stress errors asymmetrically.

II. Methodology

The goals of the study are twofold- Firstly, to verify the successful integration of the chosen model into a modern computing package. Secondly, to ascertain the usability of such a model in simulating the stress/strain response of smooth and notched members during LCF and TMF loadings. Successful integration of the model is indicated by identical response and comparison with historical data sources. Model adaptability to TMF is determined by comparisons with newly gathered data. Each of the processes in the methodology are outlined in the following subsections.

A. Material Selection

Type 304 stainless steel was an ideal candidate for this particular study for three primary reasons: Firstly, this grade of austenitic steel is widely used in a number of industries under a variety of conditions. These include high temperature isothermal and thermomechanical fatigue cycling in propulsion, energy, and petrochemical applications. Secondly, the foundations of the Miller viscoplasticity model were developed with this specific alloy, so it can be expected that the behavioral constants for the material as well as the model response should be optimal. Additionally, the relative low cost and machinability of 304 SS increases the feasibility of a more comprehensive experimental scheme in ongoing studies.

Historically, 304 SS is already documented to have a number of desirable properties for high performance applications (Refs. 8, 9). Basic material behavior and isothermal strain-life data for temperatures up to and exceeding 800°C is widely available in literature (Refs. 10-13). Although lacking the toughness and oxidation resistance of nickel-based alloys, high chromium content ensures above average defense against oxidation, while significant strength is retained at such elevated temperatures (Ref. 14). 304 SS microstructure is dominated by large austenite grains that are outlined by darker carbide-heavy boundaries. Sensitization can occur with long-term application of heat, evidenced by growth of the brittle carbide deposits (Ref. 15). Also, austenite grains are significantly lengthened in worked 304 SS, leading to large increases in tensile strength with

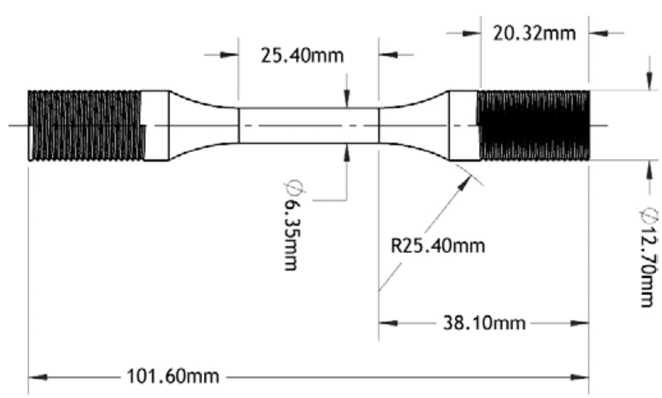

Figure 1. Test specimen geometry.

some conditioning practices. All 304 SS specimens utilized in this study were machined from annealed, as-wrought material.

B. Specimen Configuration and Testing

New experimental data for the study was gathered during mechanical testing of smooth, round, dogbone-shaped fatigue samples, with relevant specimen geometry given as shown in Fig. 1. A 100-kN MTS servohydraulic testing frame was used in conjunction with an Ameritherm HOTShot 3500W induction heating system to apply the requisite mechanical and thermal loads for the elevated LCF and TMF test types examined in the study. A general view of the experimental apparatus is shown in Fig. 2. Fully-reversed high temperature LCF tests were conducted in accordance with ASTM standard E606 (Ref. 16) at 600°C with a mechanical strain range of 0.7%, and a strain rate of 6% per minute. Specimens under these conditions exhibited noticeable isotropic hardening initially, followed by a period of softening lasting several hundred cycles before stress stabilization occurred. Thermomechanical fatigue tests were also conducted as fully reversed, with a mechanical strain range of 0.7% in both in-phase and out-of-phase configurations. In each case, a minimum temperature of 200°C and a maximum temperature of 600°C were applied. TMF tests were conducted in accordance with ASTM standard E2368 (Ref. 17). A mechanical strain rate of 0.84%/min and a matching thermal rate of 4°C/sec were employed in both IP and OP TMF tests. Specimens subjected to these thermomechanical fatigue conditions also experienced initial hardening, followed by softening and stress stabilization – albeit with overall lifetimes reduced significantly. A summary of experimental data employed in this comparative analysis are available in Table 1.

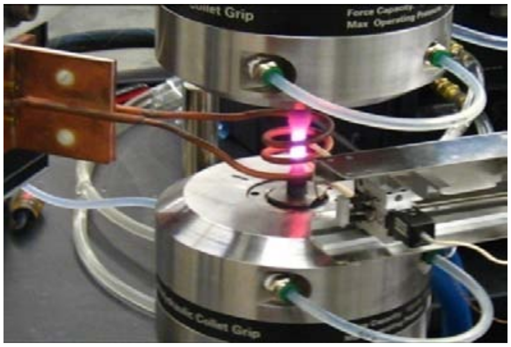

Figure 2. Test equipment configuration.

Table 1.   Experimental load cases

Load Case	Strain Ratio, R_ε	Mech. Strain Range, $\Delta\varepsilon_{mech}$	Max Temp, T_{max}	Min Temp, T_{min}	Data Source
LCF	-1	1.0%	593C	593C	Miller/Collum
LCF	-1	0.7%	600C	600C	UCF
IP TMF	-1	0.7%	200C	600C	UCF
OP TMF	-1	0.7%	200C	600C	UCF

C. Numerical Model Adaptation

Miller's 1976 viscoplasticity model has been adapted to the commercial computation package ANSYS as a user programmable feature (UPF) by the Mechanics of Materials Research Group (MOMRG) at the University of Central Florida (UCF). A Fortran 90 subroutine was implemented as a user plasticity law governed directly by the principal formulation of Miller's model, given by Eq. (1).

$$\dot{\varepsilon} = B\theta' \left\{ sinh\left[\left(\frac{|\sigma - R|}{D}\right)^{1.5}\right]\right\}^{n} sgn\,(\sigma - R) \tag{1}$$

$$\dot{R} = H_1\dot{\varepsilon} - H_1B\theta'\,[sinh(A_1|R|)]^n sgn\,(R) \tag{2}$$

$$\dot{D} = H_2|\dot{\varepsilon}|\left[C_2 + |R| - \left(\frac{A_2}{A_1}\right)D^3\right] - H_2C_2B\theta'[sinh(A_2D^3)]^n \tag{3}$$

Additionally, the subroutine also calculates a version of the characteristic drag stress, *D*, and the rest stress (also commonly known as back stress), *R*, per execution step. Miller's expressions for drag stress and back stress directly control isotropic hardening and kinematic hardening behaviors of the model (Ref. 18), respectively. The model calculates the changes in these values per time step, and the expressions are given by Eqs. (2) and (3).

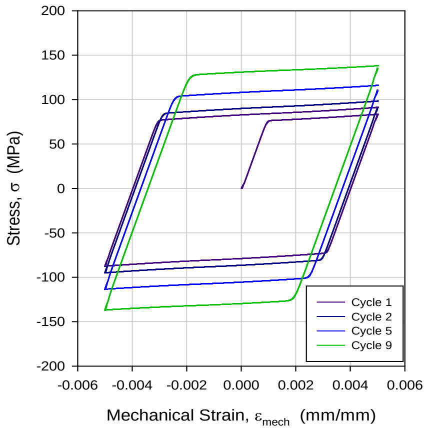

Figure 3. LCF simulation at 593°C.

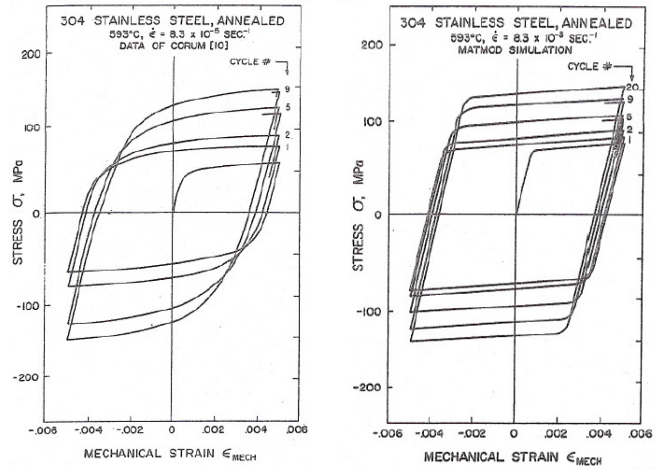

Figure 4. Comparison of 304SS LCF loading (from 2.)

During execution, material constants, behavioral constants, and boundary conditions for the solution step are handled externally by the inbuilt ANSYS code. Stress/strain states that induce plasticity transfer relevant quantities to the subroutine. Historical changes in the model response are implemented through continual updates of the resultant *R* and *D* values as state variables. Illustrated in Figures 3 and 4, the response of the modernized implementation closely matches that of the original MATMOD simulations introduced by Miller in 1976.

III. Results

Clear indicators of accuracy in the model response are found in analysis of the hysteresis loops and stress histories for varying load conditions. For given cycles, the actual stress/strain response of the material is matched against the model. Particular metrics of interest include loading and unloading moduli, the overall strain energy enclosed by the hysteresis curve, and how sudden or gradual the onset of plasticity may be. Analysis of the peak and valley stresses offers a rapid glance at how over- or under-conservative the model may be when considering successive loadings.

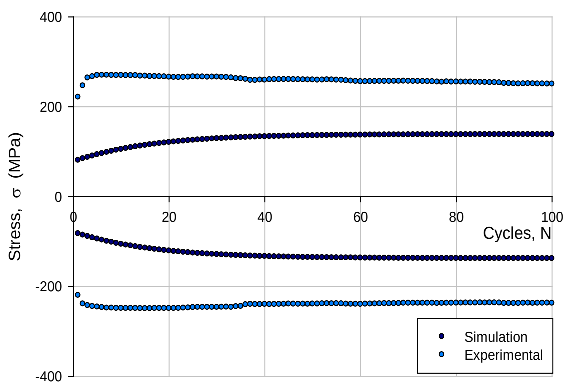

Figure 5. 600°C LCF stress history comparison.

A. High Temperature Fatigue Results

Comparison of the model's stress response for high temperature LCF with that of Corum (used by Miller in model development) reveals a reasonable qualitative fit, with decreasing isotropic hardening being the primary dynamic feature of the cyclic stress/strain response. Minimum error occurs at the peak and valley stresses for each cycle, with the model initially greatly overestimating these values. Between cycles 5 and 9, hardening effects become less severe, and the model begins consistently underestimating the peak values by between 10% and 15%. Analysis of the stress history of the model through 100 cycles shows that decreasing hardening occurs on the way to permanent stabilization in several tens of load reversals. Assessment of the model versus the UCF data in the 0.7% strain range case infers additional behavioral differences. While the model shows similar isotropic hardening over several tens of cycles before permanent stabilization, this effect gives way to continual softening after the first few cycles in experimental testing. Thus, the tendency of the model to stabilize instead of arrest and subsequently reverse the

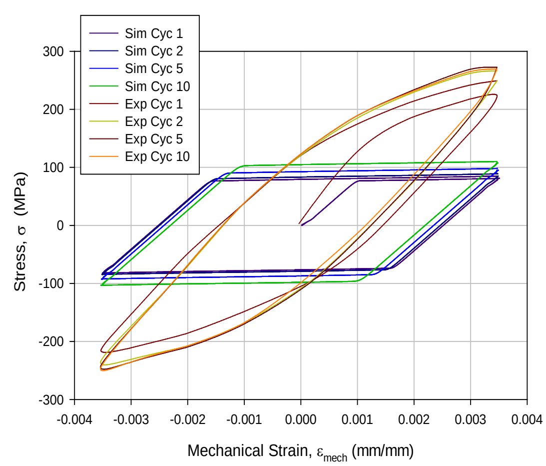

Figure 6. Cycle comparisons for 600°C LCF.

hardening altogether contributes to its overall inaccuracy in later cycles. The primary feature of the stress history comparison in the 0.7% strain range case, however, is that the Miller model simulation is significantly under-conservative in its estimate of stress response throughout the history when compared to the recent high temperature LCF data.

B. Thermomechanical Fatigue Reults

In relation to the Miller model predictions versus the LCF cases, both IP and OP TMF loads exhibited more favorable correlations with the experimental data. For the in-phase instance the model correctly predicts that

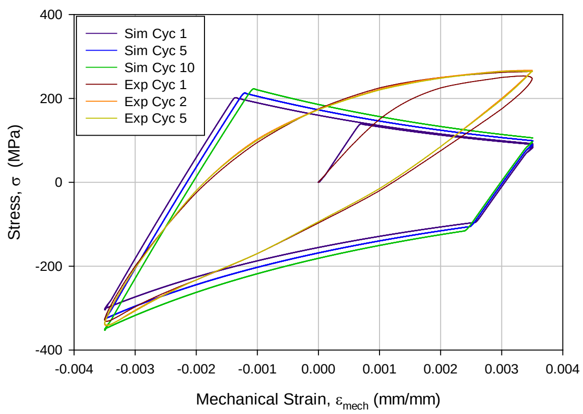

Figure 7. Cycle comparisons for IP TMF case.

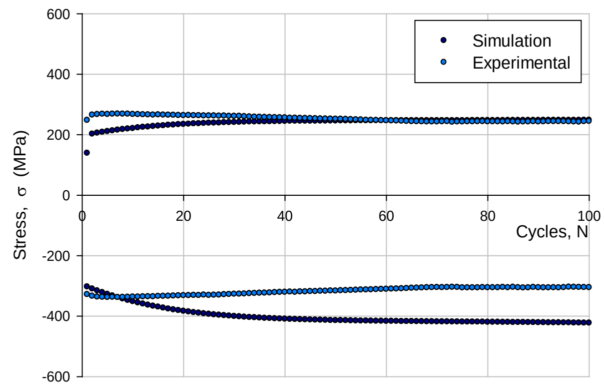

Figure 8. IP TMF stress histories.

substantial hardening will occur within the first cycle, and is in agreement with the experimental data regarding the minimum stresses per cycle. As with the LCF cases, the model predicts continually decreasing isotropic hardening before stabilizing within 100 cycles- however, the tested specimens tend to exhibit softening after the first 5 to 10 cycles. This opposition of behaviors leads to the simulation and experimental stress peaks eventually converging, while the minimum stresses per cycle settle at near 25% error. In the OP simulation run, the Miller model accurately predicted that the hardening in the initial cycles was less intensive than in other cases.

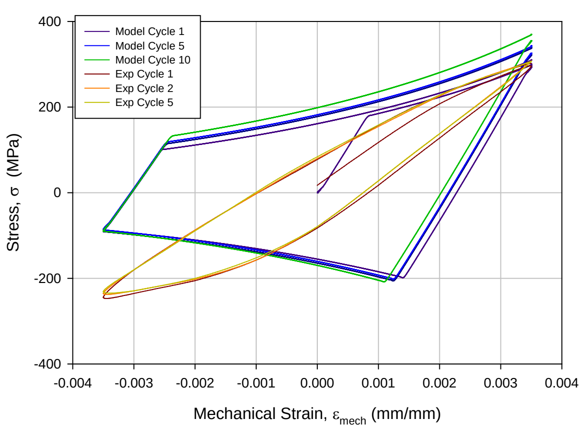

Figure 9. Cycle comparisons for OP TMF case.

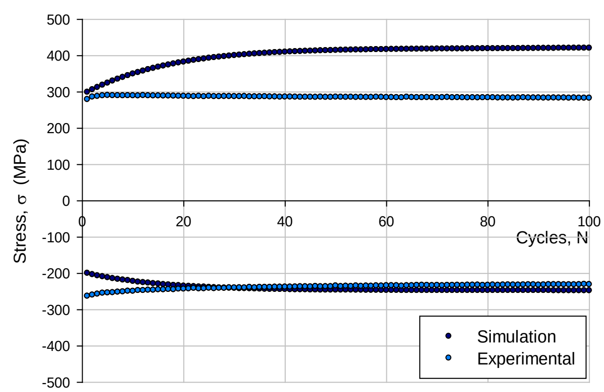

Figure 10. OP TMF stress histories.

Additionally, inspection of the stress histories reveals that the OP case shows the only noticeable evidence of kinematic hardening, occurring in the first few cycles- during this period, the Miller simulation shows asymmetric hardening response favoring the direction of the kinematic hardening. Stress minimums per cycle match closely with those of the experimental data, but as with previous cases do not occur at the same strain level. After stabilization, stress maximums are overly conservative by levels exceeding 30%.

IV. Conclusions and Discussion

In general, the reviewed model has a mixture of favorable features and shortcomings when compared with real-world behavior of type 304 stainless steel. The formulations that govern the stresses *R* and *D* provide kinematic and isotropic hardening effects to both LCF and TMF cases with levels of intensity proportionally appropriate. In the broader sense of adapting the model to non-isothermal cases, the Miller model and its handling (or lack thereof) of direct temperature dependencies was not an issue with ANSYS correctly mediating the ongoing boundary condition changes. Additionally, TMF load cases generally infer a slower mechanical strain rate versus LCF, and the difference in the UCF data was an order of magnitude in this case. Poor correlation between simulations and the UCF isothermal data yet better observed correlation with the TMF data may be indicative of a strain rate dependency effect. Mentioned in the follow-up to the original Miller paper, this sensitivity may prove to be less moderate than previously anticipated.

In order for this particular viscoplasticity model to be useful in life prediction methodologies, increased accuracy in the stress/strain states encountered well beyond the first few cycles will be necessary. Though Miller's original model was initially designed for materials that show significant work hardening, there appears to be no sufficient ability to handle eventual softening. The model itself is capable of this behavior with slowly decreasing drag stress, but it seems that the values passed from state to state are very small compared to what is necessary to affect the overall behavior. This presents a considerable shortcoming in regard to accuracy in later cycles. For every case examined during this study, hardening became qualitatively negative after only a few cycles in the test specimens, but continued on indefinitely in simulation.

Inspection of individual simulation cycles indicates general agreement with experiments in terms of hysteretic energy and stress states accompanying strain end levels. It is clear however, that the yield surface shapes differ greatly. The propensity of the simulation software to separate behavior into clear elastic and plastic regimes causes appreciable differences in response when a high level of plasticity is not encountered in the load condition.

In its present state of development, the Miller viscoplasticity model does not provide a reliable tool for determination of late TMF cycle stress/strain states. Even so, the present incarnation does serve as the basis for an adaptable constitutive model. Simple time-, rate-, and cycle-dependent terms are to be added in ongoing future development to handle the shortcomings of the present version directly. Remarks about the current state of the study and further improvements that should be considered are as follows:

1) It must be noted that adaptation of the original model to ANSYS produced slight variations in the LCF solutions when compared to the original MATMOD runs. An investigation of ANSYS versus MATMOD variable precision and solving methods may yield insight into the differences.

2) Though the Miller model does not explicitly incorporate a yield stress, it is clear that the handling code in ANSYS (and historically in MATMOD) separates the solution into simple elastic and Miller-calculated plastic regimes. In order for the yield surfaces of the model to more accurately mimic their real-life counterparts, a method which facilitates a smooth transition in simulation behavior is desired. Future iterations of development may want to attempt to incorporate a competitive parallel calculation of elastic and plastic components, or utilize a Ramberg-Osgood type of curve fit to the hysteresis response.

3) Especially for materials that easily and significantly work-harden, it seems that an explicit handling of negative hardening effects may be necessary. The current handling of the drag stress allows for this in the model, so updating Equation (3) with the inclusion of a more dominant time- or cycle-dependent term is worth consideration.

4) In non-isothermal cases, a variety of different effects occur that significantly impact the stress/strain states and cyclic lifetimes. Damage and recovery due to a wide array of mechanisms can occur with varying interaction and synergy amongst one another (Ref. 19). It is unlikely that a specific fit of TMF behavior is attainable through many cycles unless additional behavioral complexity is incorporated via functions and material constants determined by TMF testing (Ref. 20).

5) Currently, the model displays unacceptable levels of error, yet is still quite mathematically convoluted. At present, expansion of the model to multi-element or multiaxial cases should be reserved for when the previously mentioned issues are met with resolution.

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