

**ANISOTROPIC CONSTITUTIVE MODELING FOR NICKEL BASE  
SINGLE CRYSTAL SUPERALLOY RENE N4 AT 982 °C**

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Nickel base single crystal superalloys attracted considerable interest for use in gas turbine jet engine because their superior high temperature properties. In polycrystalline turbine parts, rupture is usually due to crack propagation originating at the grain boundaries. Since single crystal alloys have no grain boundaries, use of the alloy has significant advantages for increased strength and longer life.

The purpose of this paper is to report an anisotropic constitutive model developed based on crystallographic approach for Ni-base single crystal superalloy. The current equations modified a previous model proposed by Dame and Stouffer[1] where a Bodner-Partom equation with only the drag stress was used to model the local inelastic response in each slip system. Their model was considered successful for predicting both the orientation dependence and tension/compression asymmetry for tensile and creep histories for single crystal alloy Rene N4 at 1400°F. However, certain properties including fatigue were not satisfactorily modeled. In this work, a back stress state variable has been incorporated into the local slip flow equation based on the observed experimental observations. Model predictability is improved especially for mechanical properties such as anelasticity and fatigue loops. Comparison of the model predictions and the experimental data for single crystal superalloy Rene N4 at 1800°F are presented.

**MODEL DEVELOPMENT**

The application of the crystallographic approach to single crystal nickel base superalloys began with the work of Paslay et al[2], and lately by Shah[3] to the  $\gamma'$  phase of these alloys. The principal advantage of this approach is that a significant portion of the model is based on the physics of the deformation mechanisms. Presumably, this will enhance the predictive capability of the model. Furthermore, as additional information is obtained about deformation mechanisms at different loading conditions, the local constitutive models can be modified to accommodate the new knowledge.

The model developed by Dame and Stouffer[1] was based on unified theory by separating the total global strain into elastic and inelastic components. The elastic strains were calculated using cubic symmetry. The inelastic strain rate was calculated, using crystallographic approach, by summing the contributions of each slip system. The inelastic slip rate on each slip system was computed from a local inelastic constitutive equation that depends

on local resolved shear stress components in each slip direction and local state variables. Due to different mechanical responses exhibited by octahedral and cube slip systems[4,5], two separate flow equations were used to compute the inelastic strain rate on each of the two slip systems. A non-Schmid's law formulation was used to model the tension/compression asymmetry and orientation dependence in the octahedral slip system. This was achieved by incorporating the "core width effect" proposed by Lall, Chin and Pope[6] where stress-aided Shockly partials and thermally-aided cross-slip mechanisms were used to explain the tension/compression asymmetry. A Schmid's law concept was used to model the inelastic response in the cube system since tension/compression asymmetry was insignificant. In both slip systems, a Bodner-Partom type of flow equation was used to model the response at higher strain rates(i.e. tensile response). At lower strain rates(i.e. creep response), where diffusion is the controlling mechanism, a diffusion model similar to the Bodner-Partom equation was used. This constitutive model for local slip was also based on a system of state variables to model the drag stress. Back stress was not included, since this is typically associated with dislocation pile-ups at obstacles like grain boundaries which are absent in single crystals. This model was considered successful for predicting both the orientation dependence and tension/compression asymmetry for tensile and creep histories for single crystal alloy Rene N4 at 1400°F; however, properties including fatigue and anelastic recovery were not satisfactorily modeled.

The motivation to incorporate a back stress state variable in the current model was due to the fact that back stress/drag stress representation has several advantages over a drag stress model including the ability to accurately predict fatigue loops for polycrystalline materials[7,8]. However, use of these state variables has its physical background. Drag stress and back stress state variable models are used to reflect the evolution of the microstructure during deformation. Drag stress is used to approximate the resistance to inelastic flow, i.e. dislocation motions, due to obstacles such as precipitates. Generally, dislocations pass through or around the precipitates by shearing or looping mechanism. Thus the local obstacles impede the dislocation motion. Whereas, back stress is usually used to characterize the increase in resistance due to dislocation pile-ups against permanent barriers such as grain boundary, which create a repulsive stress between adjacent dislocations. It was assumed by Dame and Stouffer that back stress should not be present in single crystal alloys due to lack of grain boundaries. Thus only the drag stress was included in their model. However, it is too restrictive to assume that back stress can only be created by dislocation pile-up mechanism. For example, Milligan and Antolovich[9] showed in their study of deformation behavior of single crystal superalloy PWA 1480 that when dislocations emerged from precipitates those portions of the dislocations within the precipitate are constricted due to high anti-phase boundary energy(APBE), while those portions of the same dislocations which had exited the precipitates are split due to elastic repulsion. Therefore, it is likely that elastic repulsion, i.e. back stress, should be included in the force equilibrium equation. More generally, it is suspected that dislocation interaction and/or rearrangement will also result in creation of back stress in the single crystals[10], except the effect may be insignificant compared to

the pile-up mechanism. Thus, it was decided to evaluate the macroscopic effect of the back stress in the mechanical test.

In order to better understand how back stress affect the inelastic strain rate, the following mathematics are required. A typical drag stress/back stress model[5,6] for polycrystalline metals has the functional form as

$$\dot{\epsilon}_{ij}^I = F\left(\frac{Z}{|\sigma_{ij} - \Omega_{ij}|}\right) \text{sign}(\sigma_{ij} - \Omega_{ij}) \quad (1)$$

where  $Z$  is the drag stress and  $\Omega_{ij}$  the back stress. Based on this formulation, inelastic flow can be present even when the applied stress,  $\sigma_{ij}$  is zero, i.e. as long as the back stress is non-zero and is large enough to produce meaningful strain rates. This is normally seen in the relaxation test at zero stress. Therefore two special single crystal tests were designed and performed in the beginning of this research. The results of these tests are shown in Figure 1 and Figure 2. The predicted results in these figures will be discussed in a later section. Figure 1a and 1b shows double tensile tests on specimens in [100] and [111] orientation, respectively, with a 120 second hold time. In both tests, samples were first loaded to 1.5% strain at strain rate of  $1 \times 10^{-4}$ /sec, unloaded immediately to zero stress within 10 seconds, and following the 120 seconds hold period and then reloaded at higher strain rate of  $6 \times 10^{-4}$ /sec. Significant anelastic recovery has occurred during the hold period for the [100] sample, whereas the recovery is minimum for the [111] specimen. These results clearly demonstrate that the recovery mechanism is orientation dependent. Second, without the presence of back stress term similar to equation (1), a single drag stress formulation cannot predict this anelastic behavior. Thus, modification of Dame and Stouffer's model to include a back stress variable is necessary.

## EXPERIMENTAL PROGRAM

All the mechanical tests were performed on a MTS mechanical test unit with a 20,000 kip load frame. The tests were run under total strain control at 1800°F. The control of the MTS unit and data collection were done by computer, with software generated at the University of Cincinnati. To date, five different types of tests have been performed and five nominal crystal orientations were used. The five tests were: 1) monotonic tensile; 2) double tensile with wait period at zero stress; 3) fully reversed fatigue; 4) fatigue with a tensile hold time in each cycle; and 5) fatigue with a compressive hold time in each cycle. The five orientations were: [123], [011], [012], [001] and [111].

## RESULTS

Shown in Figure 3 are comparisons of experimental data and predicted responses of tensile tests ran at  $1 \times 10^{-4}$  (in/in)/sec for different specimen

orientations. The responses in [100] and [111] were used to determine material constants and the response in [110] orientation was the predicted result. The model predicted well in elastic moduli, hardening characteristics (the knee part) and the saturated values for these orientations. Predictions of double tensile tests with hold time in [100] and [111] orientations are shown in Figure 1 and 2, respectively. The model predicted very well in both cases not only for the recovery part but also the hardening characteristics of the subsequent loading and rate sensitivity effect.

Experimental results showed that fatigue tests in [100], [111] and [123] orientations at 1800<sup>o</sup>F stabilized within 5 loops and exhibited no work hardening or softening throughout the lives, therefore drag stress remained constant and the evolution equation was not used. The only information used from the experimental data in determining constants was the ratio of yield stress in tension and in compression. The predictions of the loops are purely based on constants determined from the tensile tests. These predictions are shown in Figure 4 and Figure 5 for [100] and [111] orientations, respectively. In Figure 4, the model predicted very well in tension/compression asymmetry, hardening characteristic and rate effect for the [100] orientation. However, tension/compression asymmetry disappeared in Figure 5 for the [111] orientation, which the model also predicted well.

#### CONCLUSION

An back stress/drag stress constitutive model based on crystallographic approach to model single crystal anisotropy is presented in this paper. Experimental results has demonstrated the need for back stress variable in the inelastic flow equations. Experimental findings also suggested that back stress is orientation dependent and controlling both the strain hardening and recovery characteristics. Due to the observed stable fatigue loops at 1800<sup>o</sup>F, drag stress is considered constant for this temperature. The constitutive model operated with constants determined only from tensile data was extensively tested from simple tensile, fatigue to complicated stress and strain hold tests. The model predict very well in those conditions. Future works on test at other temperatures will be conducted. It is expected some strain hardening or softening of the single crystals in cyclic tests should occur.

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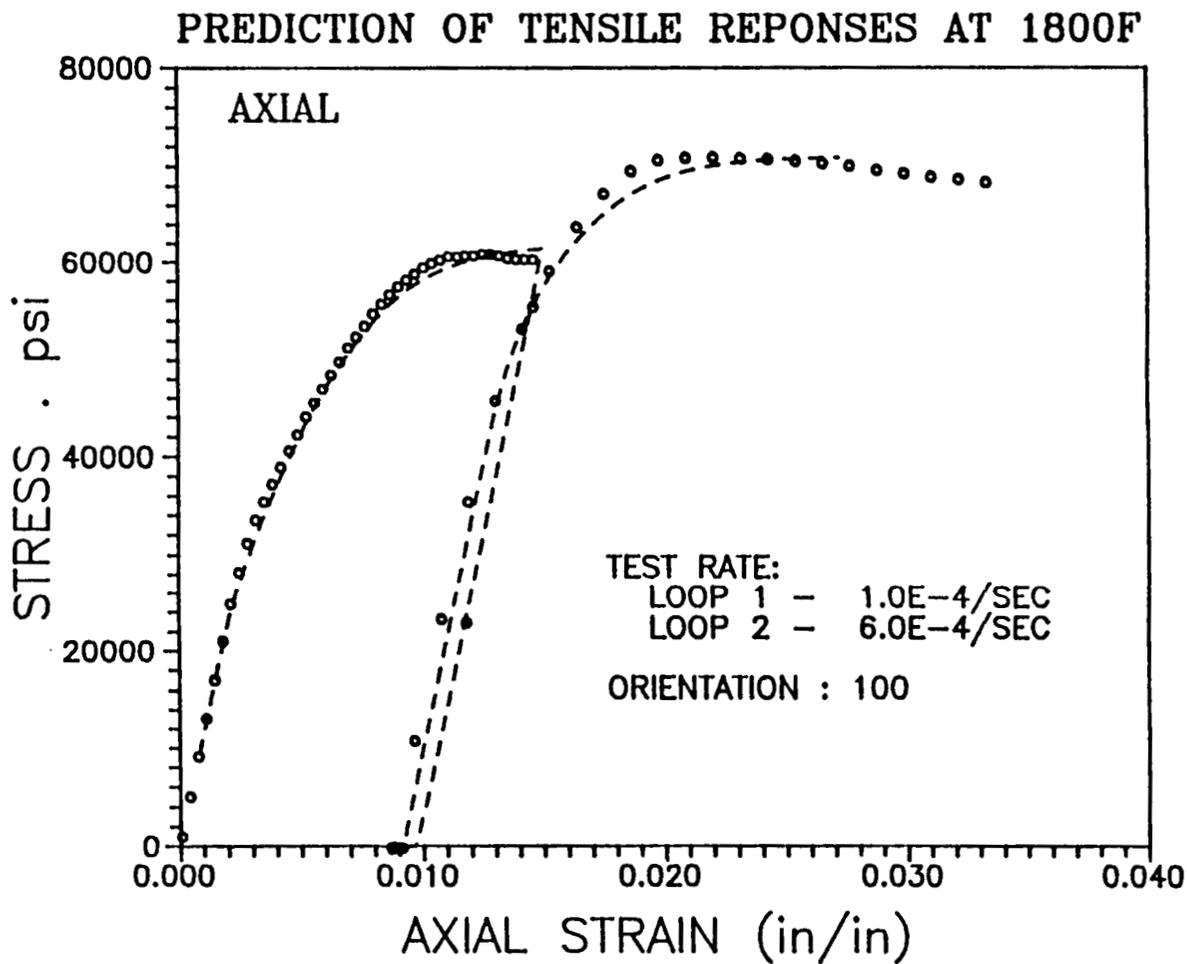


Figure 1. Predicted Response and Experimental Data for a Multiple Tensile Test in (100) Orientation with 120 seconds Hold Period. Notice significant recovery (anelasticity) during Hold Period. (RENE' N4 at 1800° F)

# PREDICTION OF TENSILE REPOSSES AT 1800F

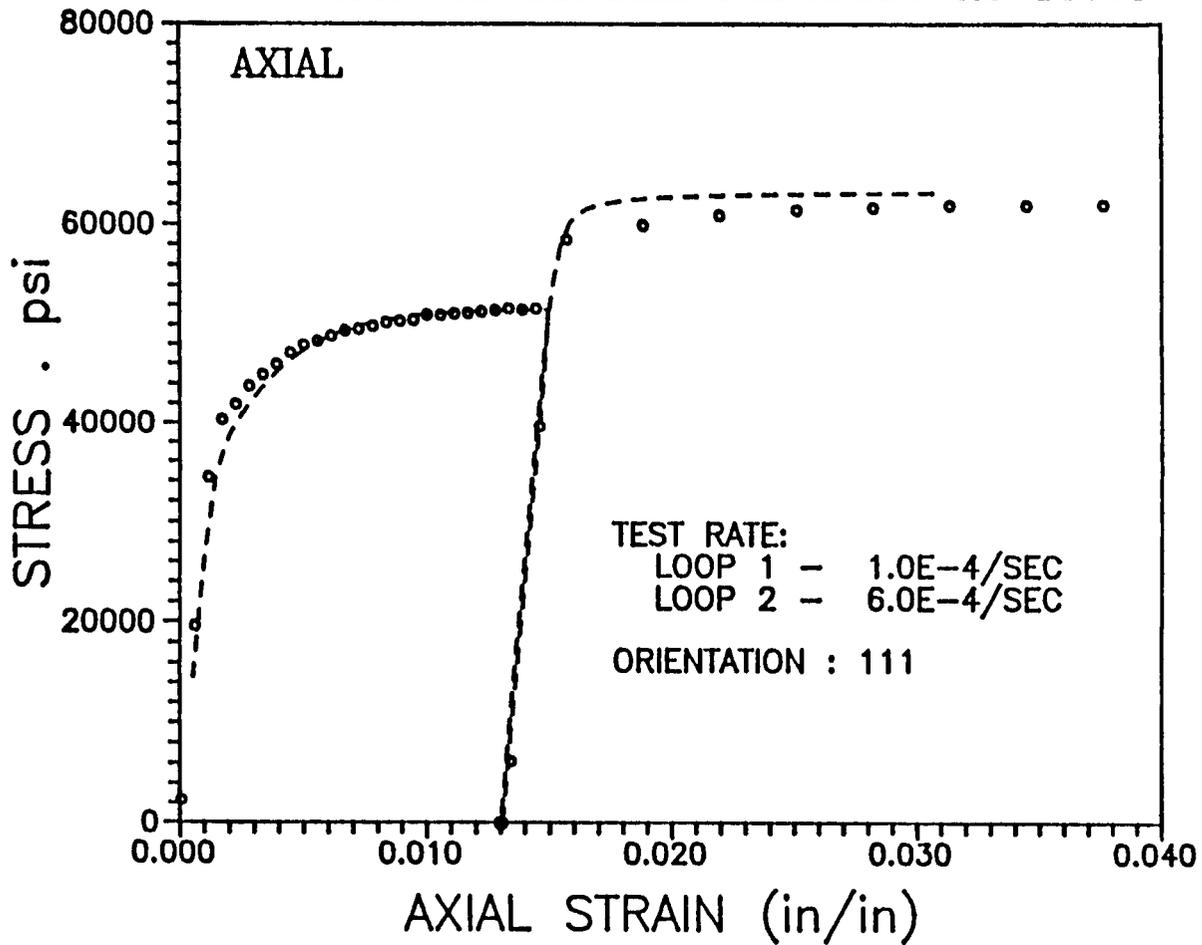


Figure 2. Predicted Response and Experimental Data for a Multiple Tensile Test in (111) Orientation with 120seconds Hold Period. Notice no recovery (anelasticity) during Hold Time.

### PREDICTION OF TENSILE REPOSSES AT 1800F

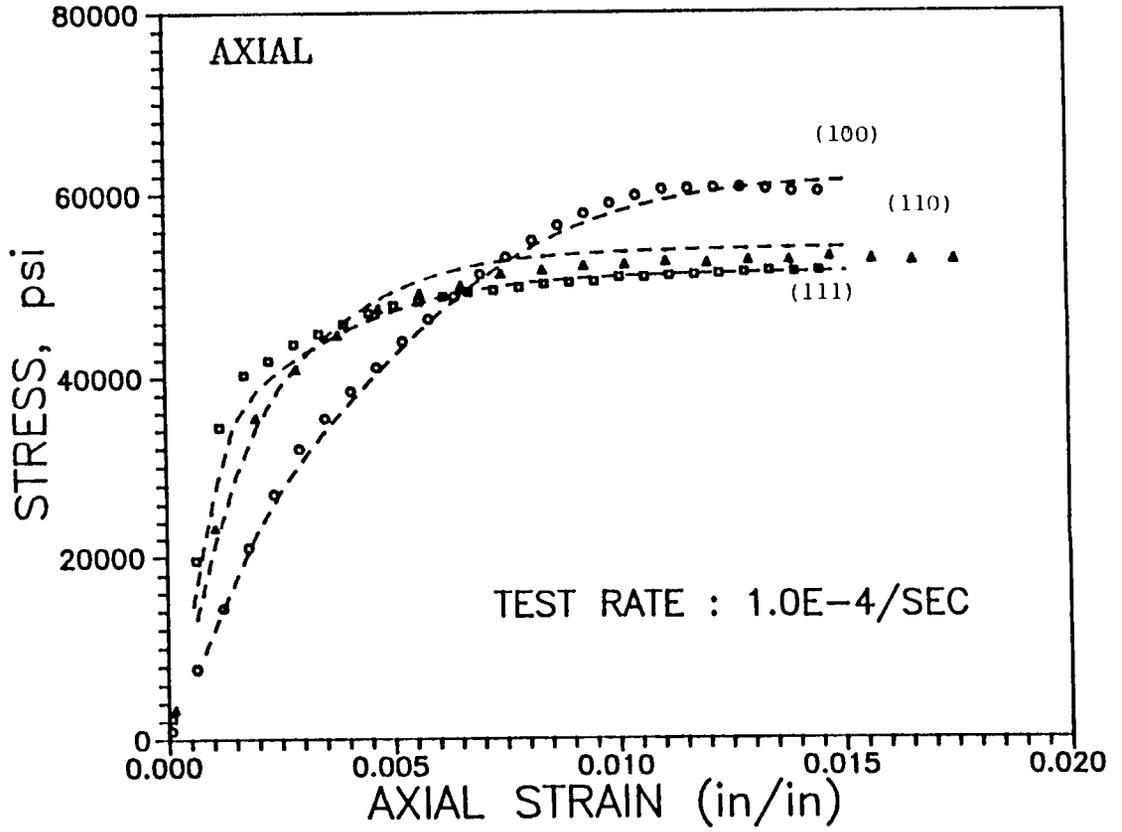


Figure 3. Predicted Tensile Responses and Experimental Data for Specimens in (100), (110) and (111) Orientation, RENE' N4, 1800° F.

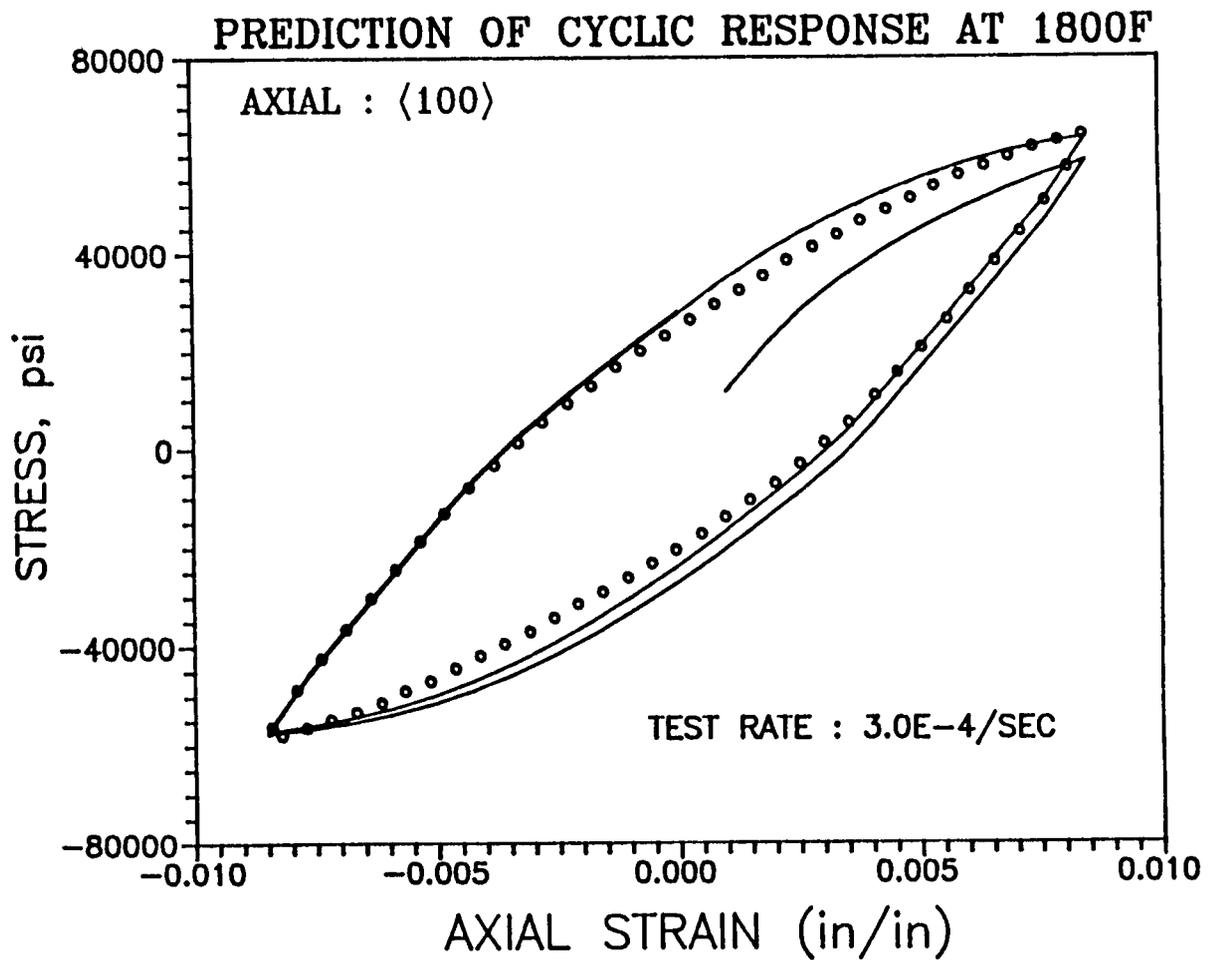


Figure 4. Predicted Response and Experimental Data for Cyclic Test in (100) Orientation, RENE' N4, 1800°F.

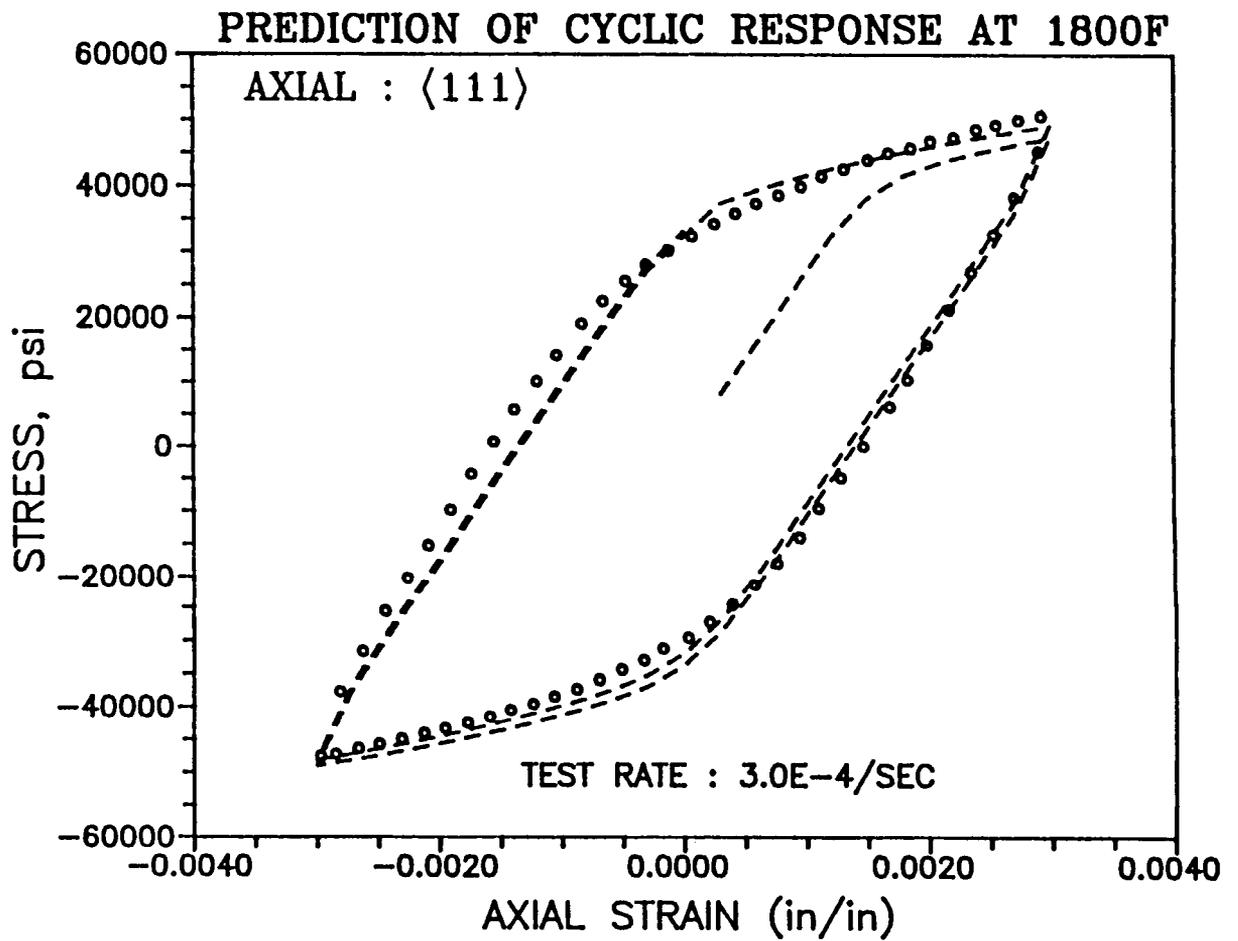


Figure 5. Predicted Response and Experimental Data for Cyclic Test in (111) Orientation, RENE' N4, 1800°F.