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PROGRESS REPORT ON CONSTITUTIVE MODELLING OF SINGLE CRYSTAL AND DIRECTIONALLY SOLIDIFIED SUPERALLOYS*

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INTRODUCTION

The trend towards improved engine efficiency and durability places increasing demands on materials that operate in the hot section of the gas turbine engine. These demands are being met by new coatings and materials such as single crystal and directionally solidified nickel-base superalloys which have greater creep/fatigue resistance at elevated temperatures and reduced susceptibility to grain boundary creep, corrosion and oxidation than conventionally cast alloys.

This report discusses work carried out as part of a research program aimed at the development of constitutive equations to describe the elevated temperature stress-strain-time behavior of single crystal and directionally solidified turbine blade superalloys. The program involves both the development of suitable constitutive models and their verification through elevated temperature tension-torsion testing of single crystals of PWA 1480.

DISCUSSION

Two types of constitutive models have been developed to describe the deformation behavior of single crystal and directionally solidified superalloys. The first type makes use of a macroscopic continuum mechanics approach in which unified viscoplastic constitutive relations are developed for materials which exhibit cubic and transversely isotropic anisotropy. A second type uses crystallographic slip theory in an attempt to model the metallurgical processes governing the deformation behavior of single crystal and directionally solidified alloys.

The macroscopic models have the advantage of requiring relatively few material constants and they can be rapidly integrated over a given strain-time history. We have found, however, that they do not represent the deformation behavior of single crystal alloys as accurately as the micromechanical formulations based on

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crystallographic slip theory. For example, the best correlation between theory and test results has been obtained by using a unified constitutive model in which the equilibrium stress (back stress or kinematic stress) hardens with inelastic strain in an anisotropic manner; that is, the equilibrium stress increments harden with inelastic strain increments through a fourth order tensor which exhibits cubic symmetry for the single crystal and transversely isotropic symmetry for the directionally solidified superalloys. This model gives reasonable predictions of the high temperature cyclic deformation behavior of single crystal specimens whose axes are oriented in the 001 and $\bar{1}11$ directions, since the material constants in the model were derived from specimens oriented in these directions. We have not yet tested the macroscopic model to predict the cyclic deformation behavior of specimens oriented in the 011 direction or to compare with the torsional behavior of specimens oriented in the 001 direction, but such comparisons are in progress.

The second type of model is based on crystallographic slip theory. Each slip system in the material is assumed to shear according to a unified viscoplastic constitutive relation. At temperatures below 750°C the single crystal alloy PWA 1480 deforms by octahedral glide of its crystallographic planes, while cube slip becomes an increasingly important deformation mode at temperatures above 750°C. We have found that both slip systems are required to model the constitutive behavior of PWA 1480 at 1600°F. The material constants for octahedral slip can be found by axial tension–compression testing of tubular specimens oriented in the 001 direction. This induces no cube slip in the specimens since the resolved shear stress promoting slip on the cube crystal planes is zero for axial tension–compression tests. The material constants for cube slip are then obtained by testing the 001 oriented tubular specimens in torsion, since this induces slip on both the octahedral and cube crystallographic planes. The cube constants may also be obtained from axial tension–compression testing of specimens oriented in the 011 and $\bar{1}11$ directions, since these tests also activate both the octahedral and cube slip systems. We have found that the material constants obtained from 001 and $\bar{1}11$ axial tests allow an accurate prediction of the axial behavior of 011 oriented specimens.

A model for directionally solidified alloys has been derived by embedding the single crystal formulation in a transversely isotropic self–consistent theory. This model has not yet been tested due to the lack of an experimental data base.

RESULTS

1. Single crystal viscoplastic constitutive models based on both macroscopic continuum mechanics and on crystallographic slip theory have been formulated and programmed as FORTRAN subroutines suitable for inclusion in the MARC nonlinear finite element program. Adapting the routines to other nonlinear codes is a trivial exercise.

2. Directionally solidified viscoplastic constitutive models based on both macroscopic continuum mechanics and on a self–consistent theory have been formulated, but

have not yet been tested or programmed due to the lack of a suitable experimental data base.

3. The macroscopic single crystal model is not as accurate as the model based on crystallographic slip theory. An anisotropic equilibrium stress state variable is needed in the macroscopic formulation to model the cubic anisotropy inherent in single crytal superalloys.

4. Both octahedral and cube slip systems are needed to model the deformation behavior of PWA 1480 single crystals at 1600°F. When the material constants are obtained from 001 axial tests and from either 001 torsion tests, or from $\bar{1}11$ axial tests, the model predicts accurate deformation behavior in the 011 tests. Predictions of axial strain rate dip tests for specimens oriented in the 001 direction are also of acceptable accuracy as shown in Figures 1–3.

5. Yield stress asymmetry is observed in PWA 1480. At temperatures below 750°C the yield stress asymmetry can be predicted according to the cross–slip theory of Takeuchi & Kuramoto, and by the Shockley partial constriction theory of Lall, Chin, Pope, Ezz, Paidar, Shah & Duhl. However, at 1600°F and above the preceding theories do not work. At temperatures below 750°C the preceding theories are in accord with the experimental results in showing that the yield stress in tension exceeds that in compression in the 001 corner of the stereographic triangle, with the reverse being true in the 011 and $\bar{1}11$ corners. At 1600°F and above, the yield stress in compression exceeds that in tension in all three corners of the stereographic triangle at strain rates above 10^{-4} sec^{-1}. The yield stress asymmetry also exhibits a strong rate dependence in which the yield stress is larger in tension than compression at low strain rates but is smaller at high strain rates. This dependence of the asymmetry on strain rate increases with increasing temperature, but cannot be modelled at present.

6. The material constants obtained from hysteresis tests at strain rates exceeding 10^{-6} sec^{-1} cannot model the deformation behavior observed in long term creep tests where the secondary creep rate is less than 10^{-7} sec^{-1}. It was hoped that this would not be the case. Leverant et al have proposed that primary creep occurs due to the dislocation motion of <112> slip systems on the octahedral {111} planes and that secondary creep occurs due to dislocation motion of <110> slip systems on the {111} planes. The present model cannot predict the long term secondary creep behavior based on the octahedral glide of the <110> systems. Possibly the <112> slip systems operate in both primary and secondary creep and we are investigating this behavior.

7. An experimental arrangement has been built and is now operational which allows biaxial tension–torsion experiments to be conducted under thermomechanical loading conditions. The software to input any given strain–temperature history has also been written and is now in operation. Experimental results are stored directly on floppy diskettes which can be used to drive the software for determining the material constants in the constitutive models.

8. In the last reporting period the material constants were determined by using the general purpose nonlinear optimization code CONMIN. A more suitable approach is now used in which the material constants are determined by a nonlinear least squares program developed specifically by the authors to determine material constants from experimental data files. This program requires the constitutive model to be integrated over the strain histories in the experimental data files, and the nonlinear least squares approach necessitates the use of an iterative technique. Because of the large amount of integration required it is necessary to integrate the single crystal constitutive model very rapidly. This is accomplished by casting the complicated three dimensional form of the model into three much simpler models which are suitable for the axial integration of specimens oriented in the 001 and $\bar{1}11$ directions, and for the torsional integration of specimens oriented in the 001 direction.

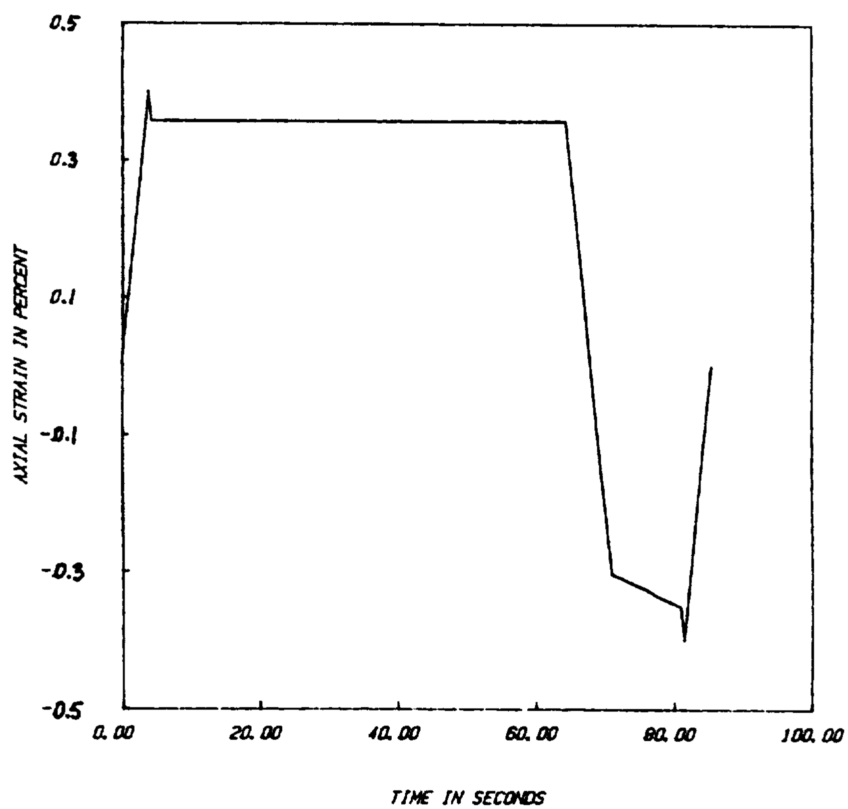

Fig 1. Experimental Strain-Time History For Dip Test On PWA 1480 at 1600F

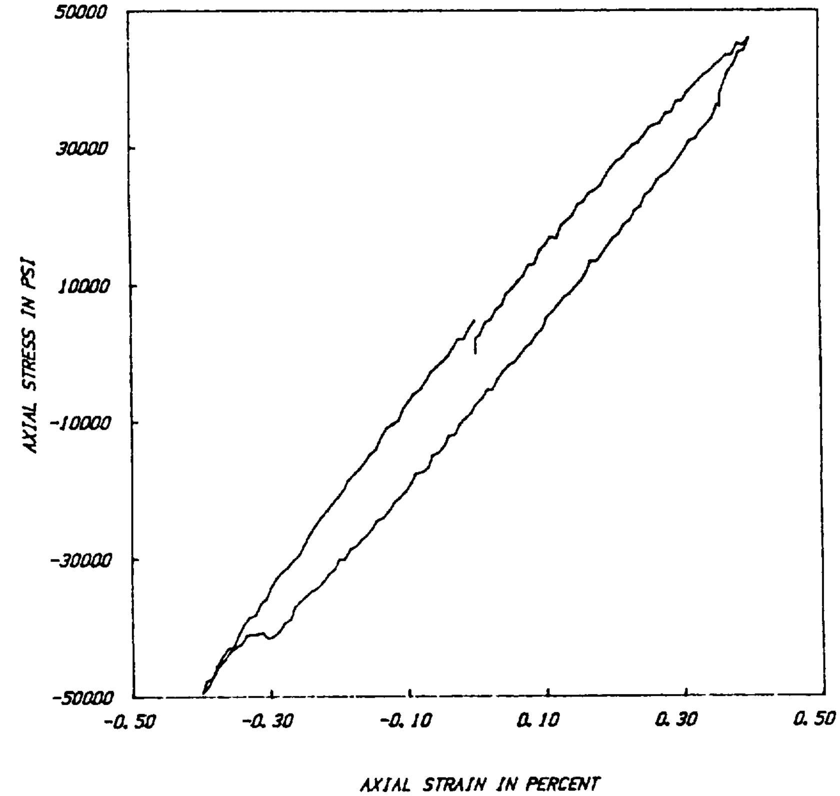

Fig 2. Experimental Stress-Strain Loop During Dip Test On PWA 1480 at 1600F

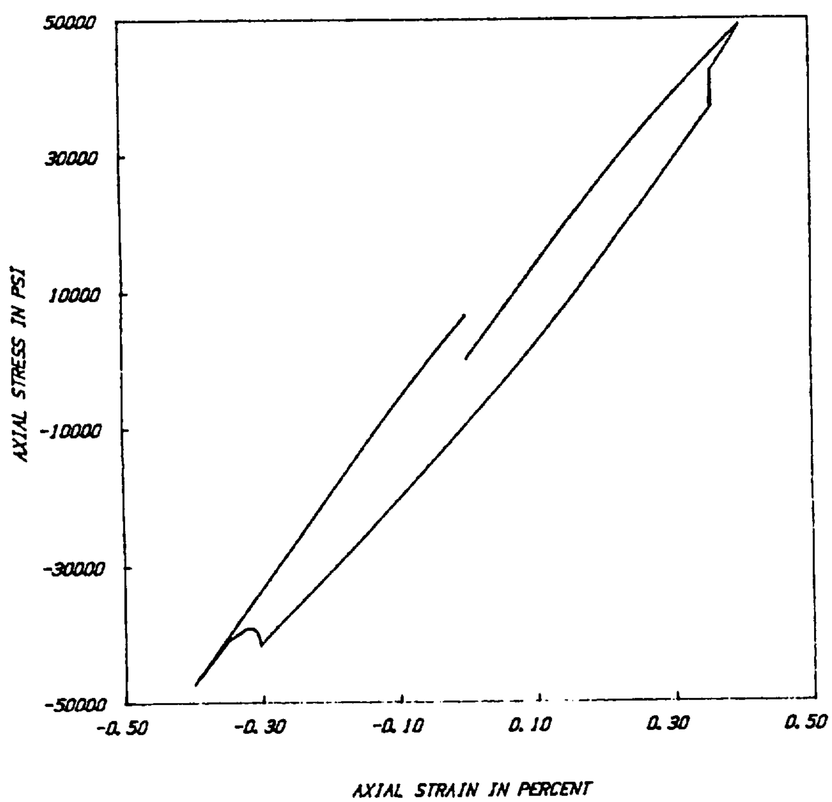

Fig 3. Predicted Stress-Strain Loop During Dip Test On PWA 1480 at 1600F