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CONSTITUTIVE MODELING OF INELASTIC ANISOTROPIC

# MATERIAL RESPONSE

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## INTRODUCTION

The broad objective of this research program is to develop a constitutive equation to predict the inelastic thermomechanical response of single crystal superalloys. These equations are essential for developing accurate finite element models of hot section components and contribute significantly to the understanding and prediction of crack initiation and propagation. The specific goal is to develop a WORKABLE constitutive equation for single crystal turbine blades that can be used in a finite element model for structural analysis.

The method used in this program is limited to unified state variable constitutive equations. Unified equations are valid over the entire deformation history and do not require separate representations for loading and unloading. State variables are employed in an attempt to characterize to essential features of changes in the material microstructure during the deformation history.

Two approaches to developing an anisotropic constitutive equation have been reviewed in detail. One approach is to apply the Stouffer-Bodner [1,2] representation for deformation induced anisotropy to materials with an initial anisotropy such as single crystals. This representation is developed in the eigenspace of the stiffness or compliance matrix to eliminate coupling so that one component of stress produces only one component of strain rate. The second approach is to determine the global inelastic strain rate from the contribution of the slip in each of the possible crystallographic slip systems (Pasley et al [3,4]). In each of these representations the model of Bodner et al [5,6,7] for isotropic materials is used to characterize the fundamental slip mechanisms. This representation is based on the Prandtl-Reuss flow equation an has one state variable to characterize both strain hardening and thermal recovery. A three dimensional finite element is being developed with a variable constitutive equation link that can be used for constitutive equation development and to predict the response of an experiment using the actual specimen geometry and loading conditions.

## THE EIGENSPACE APPROACH

The form of the deformation rate equation used in [1,2] was an extension of the Prandtl-Reuss flow equation of classical plasticity to allow anisotropy. The equation related the inelastic strain rate vector,  $\varepsilon_{\alpha}^{I}$ , to the deviatoric stress vector,  $S_{\alpha}$ , by a six dimensional second order linear transform whose components are functions of stress and stress history; i.e.,

 $\hat{\epsilon}^{\mathrm{I}}_{\alpha} = \lambda_{\alpha\beta} S_{\beta}$  ( $\alpha, \beta = 1 \text{ to } 6$ ) (1)

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where  $\lambda_{\alpha\beta}$  is constrained to satisfy incompressibility. Equation (1) reduces to the isotropic flow rate if  $\lambda_{\alpha\beta}$  is replaced by a scalar material function.

In general, the flow equation (1) has both normal and shear stress coupling. That is, one component of stress can produce six components of inelastic strain rate. However, if Equation (1) is transformed to the eigenspace of the compliance tensor; i.e.,  $\lambda_{\alpha\beta}$  is diagonal, then the coupling is eliminated. This implies that

one component of stress will only produce one component of inelastic strain rate. The technique produces an extremely simple and mathematically convenient flow rule. Further, the eigenspace formulation has been used to propose a number of different hardening rules.

However, the transformation matrix that carries  $\lambda_{\alpha\beta}$  into the eigenspace must

also be determined as part of the constitutive formulation. In general it is expected that this transformation matrix would contain information of the anisotropy of the material and, therefore, depend upon the deformation history. Thus, in a material with initial cubic symmetry, for example, it is expected that the deformation itself will alter the cubic response through cross hardening and the Bauschinger effects. In this case the initial cubic symmetry cannot be imposed during the entire response. Calculations have shown that for an incompressible cubic material the transformation between the physical space and eigenspace is constant and independent of the material parameters; however, for more complex symmetry, such as orthotropic the transformation matrix depends on the deformation. Thus, the components of the transformation matrix must also be determined from the experimental data. This has caused some difficulty because the material parameters (transformation matrix components) are mathematically motivated rather that physically motivated.

### THE CRYSTALLOGRAPHIC APPROACH

The orientation, temperature and stress dependence of the deformation of single crystal superalloys can also be modeled by analyzing the deformation on each of the crystallographic slip planes and summing the results. This approach can be developed from the actual deformation mechanisms present in the material and should lead to a better understanding of underlying physical phenomena.

The typical microstructure of a nickel-base single crystal superalloy, Mar M200 for example [8], contains fcc  $\gamma^1$  distributed in a fcc  $\gamma$  solid solution matrix. The microstructure also contains MC carbides and micropores in the interdendritic regions. The matrix can exhibit both <110> and <112> slip on the octahedral planes, [111], and the  $\gamma^1$  can exhibit slip on both the octahedral and cubic, [100], planes. Further planer and wavy glide and dislocation climb have been observed in at the temperature range of interest. Thus, several slip systems and several deformation mechanisms can be active in the range of thermomechanical loading present in gas turbines.

An appropriate starting point is to base the modeling on Schmid's law; i.e., the slip in a crystallographic slip direction on a slip plane is a function of the shear stress component in that slip direction. This is a valid assumption for <011>

slip on the octahedral planes in Mar M 200 at  $760^{\circ}$ C but not at  $870^{\circ}$ C, [8]. The relationship should also depend on the current material microstructure and temperature to include the important response properties. Schmid's law has been formulated in a mechanics context by Pasley et al [3,4]. In this work the total inelastic strain rate tensor is constructed by transforming the strain rate on each

of the slip directions into the crystallographic basis and summing over all slip directions. The linear superposition is valid since strain can be represented by a linear transform. Modifications to this approach include replacing the simple creep representation used in [3,4] by a constitutive equation [5,6,7] to include history dependence. It is also necessary to determine the active slip systems and deformation mechanisms as a function of temperature and strain rate to correctly characterize the material. Methods must also be included to account for cross hardening within each material phase and the interaction between the  $\gamma$  and  $\gamma^1$  material phases. Finally the phenomena associated with thermal cycling must be identified and modelled.

#### FINITE ELEMENT MODEL

A finite element code is being developed that incorporates a time dependent constitutive model based on octahedral and cube slip. There are a number of possible flow rules, hardening rules and cross hardening rules. These are being incorporated into the FEM code so that they can be studied in various combinations in depth. An important part of the constitutive model development will involve an experimental - finite element analysis - constitutive model verification loop. Since a limited amount of instrumentation is possible during specimen testing an important part of constitutive model verification will involve a comparison between the deformed specimen dimensions and the FEM analysis.

The finite element code being developed uses twenty noded isoparametric bricks and an initial strain iterative procedure. The inelastic response is computed at each of the order two Gauss quadrature points. Since relatively small inelastic strains are expected in actual material applications small strain and small displacement theory is used. Additional features of the finite element code are the ability to model piecewise linear load histories and a dynamic time incrementing procedure.

As it is now being developed this finite element code is intended for use as a tool in constitutive model development. However, with a few relatively minor modifications the code should be useful as an analysis and design tool.

#### PLANS AND PROBLEMS

During the next year we plan to continue development of the constitutive models with emphasis on the crystallographic approach. It is hoped that these studies may also provide some insight into determining the material functions in the eigenspace approach. Further success depends on our ability to identify the active slip systems and deformation mechanisms present in the material. For example, at the present time three slip systems containing a total of 30 slip directions have been identified. Assuming positive and negative slip to be different gives 60 stress and strain rate variables. If each slip system can exhibit three mechanisms then nine sets of constitutive parameters are required. Thus, an extensive number of variables and material parameters can be brought into the formulation. To avoid curve fitting a careful plan must be established to evaluate and assemble the constitutive model. This should include an experimental program at the crystallographic level to identify the active slip systems and deformation mechanisms in the material system of interest and use these results to determine atleast some of the constitutive parameters.

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