CONSTITUTIVE MODELLING OF SINGLE CRYSTAL AND DIRECTIONALLY SOLIDIFIED SUPERALLOYS*

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Nickel-base monocrystal superalloys have been under development by turbine manufacturers for a number of years. Successful attempts have now been made under grant NAG3-512 to the University of Connecticut to model the deformation behavior of these materials based on both a macroscopic constitutive model and a micromechanical formulation based on crystallographic slip theory. These models have been programmed as FORTRAN subroutines under contract NAS3-23939 to Pratt & Whitney and included in the MARC nonlinear finite element program. They are currently being used to simulate thermalmechanical loading conditions expected at the "fatigue critical" locations on a single crystal (PWA 1480) turbine blade. Such analyses form a natural precursor to the application of life prediction methods to gas turbine airfoils.

SINGLE CRYSTAL FORMULATIONS

The difficulty in analyzing the deformation behavior of single crystal materials lies in their anisotropic behavior. Two separate unified viscoplastic constitutive models for monocrystal PWA 1480 have been completely formulated. In one model the directional properties of the inelastic deformation behavior are achieved by resolving the summed crystallographic slip system stresses and strains onto the global coordinate system. In the other model the required directional properties are achieved by operating on the global stresses and strains directly with fourth rank anisotropy tensors. The crystallographic slip based model is more accurate and has more physical significance than the macroscopic model, but is more computationally intensive than its macroscopic counterpart.

The material constants in both models can be obtained from uniaxial tests on <001> and <111> orientated uniaxial specimens, or from uniaxial and torsion tests on <001> orientated tubular specimens. Both models achieve good correlation with

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* Work performed under NASA grant NAG3-512
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the experimental data in the <001> and <111> corners of the stereographic triangle, and both models correctly predict the deformation behavior of specimens orientated in the <011> direction. In grant NAG3−512 the tension−torsion tests on tubular specimens orientated in the <001> direction were carried out at a temperature of 1600F at the University of Connecticut. Further tests at temperatures ranging from room temperature to 2100F have been carried out at Pratt & Whitney under contract NAS3−23939. Good correlations and predictions are uniformly achieved at temperatures above 1200F, but further work appears to be necessary to correctly model the deformation behavior of PWA 1480 monocrystal material below 1200F.

MATERIAL CONSTANT DETERMINATION

The determination of the material constants in anisotropic monocrystal materials poses many difficulties and is greatly facilitated by using an iterative nonlinear least squares program. If x_m denotes the vector which contains the material constants, the computed stress will depend on the material vector x_m and can be written as $\sigma(x_m)$, where m ranges from 1 to N, with N being the number of material constants in the vector x_m. The test result corresponding to the computed value of $\sigma(x_m)$ is denoted by σ^T.

The material constant vector x_m can be determined by minimizing the square of the difference between the test results and the computed results at the user selected points 1, 2, ... , M in the experimental data files. The total number of experimental points in the experimental data files is usually much larger than M.

In the minimization procedure the function to be minimzed is then

$$U=\sum_{r=1}^{M}\left(\sigma_r(x_m)-\sigma_r^T\right)^2.$$

If x_m^G denotes an estimated or guessed value for the material constant vector, this vector will not result, in general, in a minimum value for the objective function U. Let the vector which results in a minimum value be denoted by x_m. Then we can write

$$x_m = x_m^G + c_m,$$

where c_m is the amount, or correction, which must be added to the guessed value to produce the value which minimizes U. If the guessed vector, x_m^G, is close to the true vector, x_m, then the correction vector, c_m, will be small in comparison with x_m^G. By expanding the objective function into a Taylor series the correction vector can be determined by solving the system of equations

$$\sum_{q=1}^{N} A_{pq} c_q = b_p \text{ for } p = 1, 2, 3, \ldots, N,$$

where

$$A_{pq} = \sum_{r=1}^{M} \left(\partial \sigma_r(x_m^G)/\partial x_p\right)\left(\partial \sigma_r(x_m^G)/\partial x_q\right) \text{ and } b_p = -\sum_{r=1}^{M} \left(\sigma_r(x_m^G) - \sigma_r^T\right)\left(\partial \sigma_r(x_m^G)/\partial x_p\right),$$

by means of a Gaussian elimination method. Since only the first term in the Taylor series is kept in the preceding expansion, the solution vector c_m is not exact. However, it may be added to the guessed material constant vector x_m^G to obtain the improved vector

$$x_m^{\text{Improved}} = x_m^G + \beta c_m.$$

This process is repeated in an iterative manner until convergence is achieved. The parameter β is used to stabilize the method and assumes small values when the initial guess for the material constant vector is far from the true solution, and approaches unity as convergence is achieved.

The preceding iterative technique has proved to be of great value in estimating the material constants required for use in unified viscoplastic formulations. This is especially the case in anisotropic formulations where simplified means of estimating the material constants are not available.