WORKSHOP

STOCHASTIC AND MULTISCALE INVERSE PROBLEMS

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An inverse optimization strategy to determine single crystal mechanical behavior from polycrystal tests: application to Mg alloys.

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An inverse optimization strategy was developed to determine the single crystal properties from experimental results of the mechanical behavior of polycrystals. The polycrystal behavior was obtained by means of the finite element simulation of a representative volume element (RVE) of the microstructure in which the dominant slip and twinning systems were included in the constitutive equation of each grain included (basal, prismatic, pyramidal slip and extension twinning). The behavior of the grains follows a crystal plasticity model developed in [1] and implemented as a material subroutine in the finite element code ABAQUS. Kalidindi's model [2] was used for the twinning mechanism and a power-law was chosen for the viscoplastic flow (both for plastic slip rate as and evolution of twinning volume). The inverse problem was solved iteratively by means of the Levenberg-Marquardt method [3, 4], which provided an excellent fit to the experimental results. This method is based on minimizing an objective function $O(\boldsymbol{\beta})$ (1) that depends on the comparison between the experimental curves x_i, y_i and the numerical curves $f(\boldsymbol{\beta})$. The numerical curves are obtained by the finite element analysis of the RVE using the boundary conditions corresponding to the loading case simulated. The response of the polycrystalline material has a strong non-lineal dependency of a set of parameters $\boldsymbol{\beta}$ which define the single crystal behavior.

$$O(\boldsymbol{\beta}) = \sum_{i=1}^{n} \left| y_i - f(x_i, \boldsymbol{\beta}) \right| = \left\| \mathbf{y} - \mathbf{f}(\boldsymbol{\beta}) \right\| \qquad (1)$$

The new strategy was employed to identify the initial and saturation critical resolved shear stresses and the hardening modulus of the active slip systems and extension twinning in a textured AZ31 Mg alloy [5]. Also, this procedure was used in order to understand the influence that both temperature as the precipitates have on the MN10 and MN11, two Mg alloys with a small content of rare earths [6, 7].

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