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An inverse optimization strategy to determine single crystal mechanical behavior from polycrystal tests by means of computational homogenization

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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 of the microstructure in which the dominant slip and twinning systems were included in the constitutive equation of each grain [1-2]. The inverse problem was solved by means of the Levenberg-Marquardt method, which provided an excellent fit to the experimental results. The iterative optimization process followed a hierarchical scheme in which simple representative volume elements were initially used and successively by more realistic ones to reach the final optimum solution, leading to important reductions in computer time.

The new strategy was applied 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. The results were in general agreement with the data in the literature but also showed some differences. They were partially explained because of the higher accuracy of the new optimization strategy but it was also shown that the number of independent experimental stress-strain curves used as input are critical to reach an accurate solution to the inverse optimization problem. It was concluded that at least three independent stress-strain curves are necessary to determine the single crystal behavior from polycrystal tests in the case of highly textured Mg alloys.

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