Comparison of Polycrystalline Full-Field and Homogenized Models for Tantalum forming

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Abstract

Finite element simulations are invaluable for predicting microstructure evolution during manufacturing processes, which directly impacts the final mechanical properties of a part. In this context, polycrystalline models-whether full-field or homogenized-are particularly effective, as they can simultaneously predict both mechanical behavior and microstructure evolution. This capability is critical for applications such as forming of pure tantalum, a highly ductile metal, which presents significant industrial challenges for CEA.
In this study, crystal plasticity finite element simulations of pure tantalum polycrystals were performed to predict the material's mechanical response and metallurgical evolution. Both full-field (polycrystalline aggregates) and homogenized models, employing a large deformation formalism, were utilized.

A full-field elastoviscoplastic model, based on dislocation density evolution, was adapted within the finite element code Zset. This implementation was built on the model and parameters established by S. Frenois, with particular attention given to the interaction matrix between dislocation slip systems in the isotropic hardening law (1, 2,3). Additionally, a homogenized polycrystal model called β-model (1) was adapted in Zset.

To validate these models, simulations of tantalum single crystals under various loading conditions were conducted and compared to both experimental and numerical results from the literature (3,4). These results were also compared to the Abaqus implementation of the β-model by S. Frenois (1). Subsequently, full-field finite element simulations of polycrystalline aggregates were carried out and compared to results from the homogenized model in Zebulon and the β-model implemented in Abaqus. The full-field simulations successfully captured the evolution of microstructure, including heterogeneous dislocation density fields and crystallographic texture evolution.

The numerical predictions of both mechanical and metallurgical properties were validated against experimental data from previous experiments by S. Frenois and new experiments conducted at CEA Valduc.

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