A novel Crystal Plasticity Finite Element framework to study materials for fusion

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The Crystal Plasticity Finite Element Method (CP FEM) [1] is a well-established tool for modeling the microstructure and properties of materials under stress or irradiation. Oxford and the UKAEA have developed a crystal plasticity code that incorporates two distinct solvers, which alternates based on slip increments and Cauchy stress. A comparison with other CP softwares that uses a similar computational framework was done through simulations of a polycrystal using ARC-supercomputer. It was demonstrated the efficiency of the proposed approach, thanks to its multimodal structure that offers improved flexibility in addressing convergence issues.

The code supports a comprehensive range of material constitutive laws to model slip, creep, strain hardening, and back stress. Parameter optimization is carried out through the Nelder-Mead algorithm [2], enabling the development of adaptable CP FEM models tailored to new experimental scenarios.

The length scale dependence of material properties is governed by Geometrically Necessary Dislocations (GNDs) [3], which can be computed using finite element interpolation functions. These functions are linked to GND density through the Nye tensor, a rank-deficient matrix that creates a system of equations with multiple possible solutions.

Two methods for calculating GNDs are studied [4]: singular value decomposition (SVD) and Karush-Kuhn-Tucker (KKT) optimization. Both methods can cause inaccurate GND densities and excessive strain hardening, even in single-slip conditions. Therefore, it's crucial to limit GNDs to active slip systems using a slip-based threshold. This approach yielded consistent and accurate results in various deformation scenarios and outperformed traditional methods in polycrystalline materials with 25% strain.

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