Simulation of the homogenized stress-strain relation for FeCrAl alloys by improved crystal plasticity finite element method

Jingyu Zhang, Shurong Ding*

Institute of Mechanics and Computational Engineering, Fudan University, Shanghai, 200433, China

Iron chromium aluminum (FeCrAl) alloys have been considered as a promising candidate for accident-tolerant fuel (ATF) cladding materials. These alloys are still under development for further optimization of their composition and processing parameters. Traditionally, new materials are developed through the method of trial-and-error, which is time-consuming and costly. The Materials Genome Initiative (MGI) serves as an efficient idea to accelerate the advanced fabrication of new materials. One of the critical problems to implement MGI is to develop multi-scale, multi-discipline modeling method and computational simulation techniques, for obtaining the homogenized stress-strain relation to characterize the macroscale mechanical properties. In the mesoscale, it is necessary to establish the finite element model for polycrystalline materials according to their microstructures and the mechanical properties of the grains.

In this study, numerical simulation of the homogenized stress-strain relation for FeCrAl alloys is implemented by improved crystal plasticity finite element method. Crystal plasticity theory is adopted to describe the plastic deformation in each grain. A three-dimensional mechanical constitutive model for single crystals is proposed with the defined co-rotational tensors. A stress update algorithm is developed to precisely reflect the shear-rate-form mechanical constitutive relation, and it is implemented in Abaqus/Explicit using a VUMAT subroutine. Computational homogenization methods are adopted to obtain the macroscopic properties from the mesoscale stress and strain fields in the representative volume element (RVE) for polycrystalline materials. The involved models and algorithms are validated by comparing the simulation results with the experimental results for the FCC copper polycrystal. Simulation results of stress-strain curves are also compared with experimental results for FeCrAl alloys with different compositions and processing conditions. The predictions of yield strength for FeCrAl alloys with different grain sizes can agree well with the experimental results. The relationships between the parameters of shear rate model and compositions, microstructures, processing conditions are also discussed. The research results indicate that the shear rate model and the improved crystal plasticity finite element method can be adopted to achieve the multi-scale simulation of mechanical performances, for optimizing the compositions and processing conditions of polycrystalline materials. The simulation results could also provide a reference for the optimization of FeCrAl alloys.

*: To whom correspondence should be addressed.
Email: dingshurong@fudan.edu.cn, dsr1971@163.com
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