Prediction of grain boundary micro-crack initiation during cyclic deformation

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J.Hazan[1,2], M.Sauzay[1]

jerome.hazan@cea.fr

[1] DEN-Service de Recherches Métallurgiques Appliquées, CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France

[2] Universités Paris-Sorbonne - UPMC, 75005, Paris, France

Abstract

Prediction of grain boundary (GB) micro-crack initiation is a major issue to understand lifetime of ductile metals and alloys subjected to cyclic deformation. Finite element simulations of the cyclic deformation of small aggregates of various fcc metals and alloys are performed. Calculations account for (i) cubic elasticity and crystal plasticity, (ii) slip localization in PSBs and (iii) production, annihilation of vacancies within PSBs and their diffusion toward the surrounding matrix, inducing a free dilatation increasing cycle by cycle. Grain boundary micro-crack initiation is predicted using both finite fracture mechanics and cohesive zone modeling.

Main results

The classical approach for predicting GB micro-crack initiation is based on dislocation pile-ups impingement on grain boundaries [1], [2]. It often conducts to wide overestimation of stress fields and underestimation of cycles to initiate micro-cracks. Indeed, contrary to pile-ups, the PSBs thickness is finite, varying from one hundred nanometer to a few micrometers depending principally on the considered material. Numerical predictions were performed for nickel, copper and 316L SS using finite element calculations, accounting for:

i. Cubic elasticity and crystal cyclic plasticity constitutive laws, which parameters are adjusted using single crystal data provided by experimental cyclic tests ;
ii. Production, annihilation of vacancies within PSBs and their diffusion toward the surrounding matrix, inducing PSB dilatation and extrusion [3]. The parameters were previously evaluated through resistivity measurements of copper single and polycrystals cyclically deformed at very low temperature.

The continuously increasing PSB leading to GB fracture is predicted using both finite fracture mechanics and cohesive zone modeling. The effects of many microstructural parameters on GB normal and tangential stress fields are estimated, such as grain size, cubic elasticity anisotropy, crystallographic orientation and GB parameters (critical stress and energy, based on atomistic simulations). Plasticity in grains impinged by PSB is discussed in contrast to GB fracture.

Finally, a statistical evaluation of microcrack density produced during lifetime is provided.

References

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