Grain size effects in polycrystalline homogenization: strain gradient and mean-free path contributions

Javier Segurado*[1,2], Daniel Rodriguez-Galán[1], Sarra Haouala[1], Ignacio Romero[1,3], Javier LLorca[1,2]

[1]IMDEA Materials Institute, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain
Tel.: +34 91 549 34 22; Fax: +34 91 550 30 47
E-mail addresses: javier.segurado@imdea.org
Web page: http://www.materials.imdea.org

[2]Department of Materials Science, Polytechnic University of Madrid
E.T.S. de Ingenieros de Caminos, 28040 Madrid, Spain

[3]Departament of Mechanical Engineering, Polythechnic University of Madrid
E.T.S. de Ingenieros Industriales, 28006 Madrid, Spain

ABSTRACT

Crystal plasticity based finite element homogenization has become a well-established framework to link the macroscopic behavior of a polycrystal with its microstructure and the crystal behavior [1]. These models can resolve strain localization due to grain misorientation and account for the effects of grain morphology and orientation distribution using three dimensional realistic microstrucures. However, models based on standard crystal plasticity (CP) are not able to predict any dependency of the polycrystalline behavior with grain size. Experimentally, it is well known that grain refinement improves the strength being this improvement normally described by Hall-Petch type relations. On the contrary, the physical micromechanisms leading to this strengthening are not so clear and depend on the alloy composition, grain size range, grain boundary distribution, initial dislocation density, etc.

In this work, two different micro-mechanisms leading to grain size effects are implemented in physically based CP models, (i) the development of plastic strain gradients due to deformation incompatibility and (ii) the reduction of the dislocations mean free path with the distance to grain boundaries [2]. For mechanism (i) a low-order strain gradient single CP model is proposed in which the hardening rate depends on the plastic slip gradients. In this model special emphasis has been paid on a rigorous definition of slip gradients in the finite element framework. It is shown that the usual approach of computing gradients using an element local derivation strategy fails in some cases, and an alternative has been proposed based on computing the slip gradients from a global nodal smoothed slip field. To account for mechanism (ii), a physically based CP model based on the Kocks-Mecking approach is enhanced by defining a limiting mean-free path for each crystal point based on its distance to nearest grain boundary.

Both models have been used in three dimensional finite element simulations of an FCC polycrystalline material with varying grain sizes. The size effects observed using each mechanism have been obtained and the grain size and dislocation density ranges in which each mechanism is dominant has been determined.

REFERENCES

[1] A Cruzado, B Gan, M Jiménez, D Barba, K Ostolaza, A Linaza, JM Molina-Aldareguia, J Llorca, J Segurado, Acta Materialia 98, 242-253 (2015)
[2] S. Lefebvre, B. Devincre, T. Hoc, Materials Science and Engineering: A, Volumes 400–401, 150-153, (2005)