COMPUTATIONAL HOMOGENIZATION OF MICROSTRUCTURAL DAMAGE IN METALS

*** E.W.C. Coenen**1,² **, V.G. Kouznetsova**1,² **and M.G.D. Geers**¹

 $¹$ Eindhoven University of Technology,</sup> Department of Mechanical Engineering P.O. Box 513, 5600 MB, Eindhoven The Netherlands www.TUE.nl, ***** E.W.C.Coenen@tue.nl

² Netherlands Institute for Metals Research P.O. Box 5008, 2600 GA, Delft The Netherlands www.NIMR.nl

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ABSTRACT

The design of metal products and forming operations is continuously challenged by demands for costs reduction, environmental regulations, new design trends etc. This, combined with the increased utilization of advanced materials, e.g. high-strength steels and aluminium alloys, requires reliable predictions of the manufacturability and (residual) product properties after forming. Also in material separation processes, such as cutting and blanking, the trajectory of process induced cracks determines the quality of the final product, and therefore need to better understood.

This work aims at further development of the physical understanding of ductile damage and the capability to translate this understanding in predictive constitutive models. For this, microstructural modelling cells of polycrystalline material are developed to capture the relevant damage mechanisms. The damage evolution in the microstructure under a far field deformation is studied by making use of homogenization techniques. Although the metal is a stochastic heterogeneous material that in general is not periodic, it can be modelled using a large enough statistically representative microstructural cell. This is true for general non-linear material behaviour including small microcracks. However, as soon as the damage start percolating and the length of the linked up microvoids becomes significant compared to the dimensions of the microstructural cell, representativety of the microstructural cell is lost. The requirement of the separation of scales is violated and the discontinuities should become apparent at the macroscale. Therefore, it is necessary to derive enhanced scale transition relations, that do not only involve the coarse scale deformation, but also the information about the localization or discontinuities.

Computational homogenization techniques based on microstructural representative volume elements have contributed a lot in understanding the microstructural evolution of a heterogeneous materials during deformation. The classical homogenization techniques make use of either prescribed displacement, traction or both to obtain upper and lower bounds for the coarse scale constitutive response of the heterogeneous material. In the strain driven framework the prescribed displacement boundary conditions are most commonly used on the entire boundary of the microstructural cell. Due to the assumption on full separation of scales, the classical homogenization techniques do not influence intrinsic length relating the characteristic microstructural dimensions to coarse scale dimensions. Using the obtained constitutive response for engineering scale calculations leads to mesh sensitivity and for the case of damaging materials to extreme localization into zero volume bands on the macroscale.

In the last decade several techniques have been proposed that aim to regularize these issues by gradient and non-local techniques [1]. These techniques are based on a proper incorporation of additional deformation measures into the kinematical macro-micro scale transition and the delivery of a corresponding stress measure. In spite of this enrichment these methods do not solve the problem of the loss of representatively after percolation, because they still rely on the scale separation.

Because the microstructural cell represents a finite material volume, a special challenge arises when the microcrack approaches or intersects the cell boundary. This problem becomes especially apparent after percolation. To circumbent this problem Belytschko [2] proposed to locally alternate the prescribed displacement to tractions equal to the average traction on the remaining boundary. This can be regarded as a variation of a self-consistent approach, which should be solved iteratively.

To stay within a fully displacement prescribed boundary value problem here is is chosen to relieve the strong requirement of a zero averaged fluctuation field on the cell boundary, typically used in classical computational homogenization. This makes it possible for microstructural localization bands to approach and intersect the cell boundary. The additional degree of freedom of the average fluctuation field on the microstructural cell boundary is related to on the macroscopic enrichments of the macrostructural first order continuum, to allow for localization development and in the limit discontinuities at the macroscale.

The developed set of boundary conditions is applied to 3D unit cells to investigate the influence of the position of second phase particles relative to a grain boundary on the damage initiation and development. Different orientations of the grain boundary have been tested. The metal matrix is modelled with local crystal plasticity and different grains are defined by different crystallographic orientations.

REFERENCES

- [1] V.G. Kouznetsova, M.G.D. Geers and W.A.M. Brekelmans. "Multi-scale second-order computational homogenization of multi-phase materials: a nested finite element solution strategy". *Comput. Methods. Appl. Mech. Engrg.*, Vol. **193**, 5525–5550, 2004.
- [2] T. Belytschko, S. Loehnert and J.H. Song. "Multiscale aggregating discontinuities: A method for circumventing loss of material stability". *Int. J. Numer. Meth. Engng.*, In press, Available online, 2007.