

A Nonlocal Interphase Approach for Modelling Interface Failure in Complex Crystalline Microstructures

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ABSTRACT

FFT based crystal plasticity solvers are powerful tools to study the effect of microstructure on the plastic response of multiphase polycrystalline materials such as advanced high-strength steels. One of their features is that they use a regular discretisation grid, allowing one to directly feed them with microstructures characterized by (electron) microscopy. This regular grid however presents a challenge when modelling fracture events, since cracks follow arbitrary trajectories which are not aligned with the computational grid. For intra-granular cracks, a phase field approach is an appealing solution [1]. However, defects in complex metallic microstructures often nucleate at or near phase boundaries and grain boundaries. Our objective hence is to develop an FFT based methodology to model decohesion of such internal boundaries, akin to cohesive zone elements in a finite element context. Our approach is based on the concept of an interfacial band along the relevant interfaces – an interphase band. This band consists of the Fourier sampling points in the vicinity of the interfaces. Within the band, the plastic constitutive behaviour is inherited from the respective adjacent grains. In addition, to model the anisotropic kinematics of the cracking process, a damage eigen strain is introduced. The eigen strain is constructed by appropriately mapping the opening deformations (in tangential and normal modes) relative to the interfacial planes. The driving forces for these openings are the resolved tractions which act against a monotonously degraded resisting force. An essential requirement is that the predicted fracture response is objective with respect to the spatial discretization, i.e. the spacing of the computational grid. In this contribution we focus on this aspect. We show that discretisation-insensitive solutions may be obtained if one ensures that the entire thickness of the band is degraded uniformly. Two strategies are compared for this purpose: a gradient based one and one employing integral type nonlocality [2]. The details of both approaches are discussed and their performance is compared for a one-dimensional problem as well as for a more realistic two-dimensional cluster of grains.

REFERENCES

- [1] P. Shanthraj, B. Svendsen, L. Sharma, F. Roters, and D. Raabe, “Elasto-viscoplastic phase field modelling of anisotropic cleavage fracture”, *Journal of the Mechanics and Physics of Solids*, Vol. **99**, pp. 19–34, (2017).
- [2] L. Sharma, R.H.J. Peerlings, P. Shanthraj, F. Roters, M.G.D. Geers, “FFT-based interface decohesion modelling by a nonlocal interphase”, *Advanced Modeling and Simulation in Engineering Sciences*, Vol. **5**, pp. 1–17, (2018).