Modeling of Gradient-Extended Crystal Inelasticity with Grain Boundary Interaction including Decohesion

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ABSTRACT

The macroscopic constitutive properties of a polycrystalline metal depend, among other things, on the size and shape of the individual grains and on the nature of interaction along the grain boundaries. A standard way of introducing a length scale in crystal inelasticity models is by incorporating gradient variables (slip gradients) in the free energy density, which typically results in an extra set of constitutive equations (commonly denoted microforce balance in the literature, refer, for instance, to [1]). These microforce balance equations require additional boundary conditions that are thermodynamically well motivated, e.g. [2].

In addition, the corresponding interface conditions along grain boundaries must be able to account for the mismatch of crystal orientation of the neighboring grains as well as the more conventional mechanical interaction. Most importantly, it is desirable to incorporate the coupling between the gradient (microtraction) interaction and classical decohesion that is expected at sufficiently extensive macroscopic strain levels. In this presentation, we discuss the appropriate modeling framework and illustrate our approach by numerical results obtained for a Representative Volume Element of the polycrystalline microstructure utilizing the Finite Element Method. In the present contribution the crystallographic structure of additively manufactured Inconel 718 is represented [3].

REFERENCES

[1] Gurtin, M.E., A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations. *J. Mech. Phys. Solids* (2002) **50**(1):5–32.

[2] Carlsson, K., Bounds on effective response for gradient crystal inelasticity based on homogenization and virtual testing. *Int. J. Numer. Meth. Engng.* to appear (2019).

[3] Kergaßner, A. et al., Modeling of additively manufactured materials using gradient-enhanced crystal plasticity. *Comput. Math. Appl.* (2018).