Gradient Enhanced Crystal Plasticity in Additive Manufacturing
Identification of a Macroscopic Yield Criterion

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In this contribution the mechanical behavior of additively manufactured Inconel 718 (IN 718) is modeled on the meso and macro scale. Gradient enhanced crystal plasticity is utilized to capture the kinematics of crystallographic slips and grain boundaries on the meso scale. The material model is solved on a representative volume element (RVE) by means of the Finite Element Method. In order to represent additively manufactured material, the RVE is based on a numerical grain growth simulation of the solidification during additive manufacturing. Mesoscopic elastic behavior and the initial yield locus are transferred to the macro scale by numerical homogenization and used to identify the parameters for a quartic yield function which is able to capture the highly anisotropic material behavior.

1 Introduction

In additive manufacturing nearly arbitrary parts are built in a layer-wise manner, e.g. using metal powders. The powder layer is fused selectively by the energy of an electron beam, guided by electromagnetic fields. This allows for a very fast deflection and hence, very high beam velocities and different scan strategies like quasi-simultaneous exposure. This allows the resulting mesostructure to be tailor-made which may range from a columnar to an equiaxed grain structure, accordingly resulting in iso- or anisotropic mechanical behavior [1]. In order to benefit from tailored materials in the design of components, appropriate anisotropic material models are required. As a result, the identification of material parameters is experimentally very expensive. Thus, isotropic material models are often applied for process simulations, simulations of parts or topology optimization. Alternatively, in this contribution, a validated mesoscopic model has been developed, which is applied to determine the parameters of a suitable material model.

The Finite Element Method together with grain structures from numerical grain growth simulations are utilized to simulate columnar grained IN 718, a face-centered-cubic (fcc) nickel base alloy. On the mesoscale, the mechanical behavior is described by a gradient-enhanced crystal-plasticity model, allowing for relative misorientations on the grain boundaries. Computational homogenization and macroscopic experimental data are used to inversely determine elastic and plastic meso- and microscopic mechanical parameters. With this model at hand the macroscopic yield locus in the six dimensional stress space is identified as surface of constant dissipation. A quartic yield function is fitted to the obtained results. A potential application is the extension of standard topology optimization with information regarding the anisotropy of the material allowing to utilize the direction dependent difference of Young’s moduli up to factor 2 and different yield stresses.

2 Material Model and Representative Volume Element

On the mesoscale, gradient enhanced crystal plasticity and a grain boundary model that is premised on the Burger’s tensor, are applied. For a detailed overview see [2] and the references therein. All relevant equations are given in (1). The balance of linear momentum, neglecting body forces is solved at small strains by means of the Finite Element Method. The elastic behavior of the fcc material is taken into account by a cubic symmetric elasticity tensor $C^\alpha$. In crystal plasticity the kinematics of crystallographic slips are directly utilized to model the plastic strains $\varepsilon^p$ by summing over all slip systems $\alpha$ considering the dyadic product of their slip direction $a^\alpha$ and slip system normal $n^\alpha$ as Schmid tensor $p^\alpha$. The model is enhanced by considering the gradients of the crystallographic slips. A physical interpretation of the slip gradients is edge- $\rho_e$ and screw $\rho_s$ dislocation densities. For each slip system a microforce balance has to be solved. The shear stresses $\tau^\alpha$, called Schmid stress and a back stress for the spatial regularization of the slips $\varepsilon^\gamma$ as well as a shear resistance $\pi^\alpha$ contribute to the micro force balance. To avoid the search for active slip systems, a creep law premised on the hyperbolic tangent is incorporated for the slip resistance $\pi^\alpha (\dot{\gamma}^\alpha)$. The hardening term $g^\alpha$ considers self and latent hardening due to the hardening matrix $h^{\alpha\beta}$. By introducing an energy that minimizes plastic incompatibility over the grain boundaries, forces $\varepsilon^\gamma \cdot n$ are derived that act on
grain A due to the grain boundary.

\[
\begin{align*}
\text{div } \sigma &= 0 \\
\varepsilon &= \frac{1}{2} [\nabla u + \nabla u^T] = e^e + e^p \\
\sigma &= \mathbf{C}^e : e^e \\
\dot{e}^p &= \sum_\alpha \gamma_\alpha^p \mathbf{p}_\alpha^\alpha \\
\text{div } \xi^\alpha &= \tau^\alpha - \pi^\alpha = 0 \\
\rho_+ &= s^\alpha \cdot \nabla \gamma^\alpha \\
\rho_\odot &= I^\alpha \cdot \nabla \gamma^\alpha \\
\xi^\alpha &= \pi_0 [s^\alpha \rho_+ + I^\alpha \rho_\odot] \\
\tau^\alpha &= \sigma : [s^\alpha \otimes m^\alpha]^{ym} = \sigma : \mathbf{p}^\alpha \\
\pi^\alpha &= [\pi_0 + g^\alpha] \tanh \left( \frac{\gamma^\alpha}{\gamma_0} \right) \\
\gamma^\alpha &= \sum_\beta \lambda_{gb} \gamma^\beta \gamma_\beta \gamma_\beta \\
\xi_\alpha^A \cdot \mathbf{n} &= -\lambda_{gb} \sum_\beta \left[ \gamma^\beta C^{\alpha\beta}_{A\beta} - \gamma^\beta C^{\alpha\beta}_{AB} \right] \\
\xi_\beta^B \cdot \mathbf{n} &= +\lambda_{gb} \sum_\beta \left[ \gamma^\beta C^{\alpha\beta}_{BB} - \gamma^\beta C^{\alpha\beta}_{BA} \right]
\end{align*}
\]

Numerical grain growth simulations [3] are applied to generate three dimensional RVEs for the simulations. The high aspect ratio of grain diameter to -length indicates that RVEs with a constant geometry in building direction are sufficient. Consequently, cross sections of the simulated grain structures, see figure 1(a), are represented and small adjustments are made to create the necessary periodicity. One RVE for the Finite Element simulations is depicted in figure 1(b). A representative list of possible crystallographic orientations is generated by means of a large number of grain growth simulations with randomly orientated crystals in the first powder layer. During Finite Element simulations, random orientations of this list are selected for the crystals. To model the macroscopic material behavior, a quartic yield function based on [4] is utilized.

![Fig. 1:](image_url)

(a) Grain growth simulation  
(b) RVE  
(c) Yield locus

**3 Numerical results**

The mesoscopic results are transferred to the macro scale by means of numerical homogenization. In order to determine the initial yield locus of the RVE, surfaces of constant dissipation are identified in all two-dimensional sub-surfaces of the six-dimensional stress space. To overcome the limitation of the small number of 12 crystals per RVE, the results for 10 different sets of unit cell orientations employing the above mentioned representative list are averaged. Due to the symmetric regularization of yielding, see \( \pi^\alpha \) in equation (1), the RVE is symmetric with respect to tension / compression. Thus, the yield locus is point symmetric and 24 evenly distributed relations of stresses \( \bar{\sigma}_{11} / \bar{\sigma}_{33} \) with \( \bar{\sigma}_{33} \geq 0 \) are simulated. The homogenized results are employed to identify the 5 independent parameters of the quartic yield function bounded to transverse isotropy. The initial yield locus of the RVE and standard deviation as well as the the quartic yield function in the \( \bar{\sigma}_{11} / \bar{\sigma}_{33} \) subsurface are depicted in figure 1(c).

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**References**

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