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Phase-Field Modeling of Ductile Fracture Across Grain Boundaries in Polycrystals

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ABSTRACT

In this study, we address damage initiation and microcrack formation in ductile failure of polycrystalline metals. We show how our recently published thermodynamic framework for ductile phase-field fracture of single crystals can be extended to polycrystalline structures. A key feature of this framework is that it accounts for size effects by adopting gradient-enhanced (crystal) plasticity. Gradient-enhanced plasticity requires the definition of boundary conditions representing the plastic slip transmission resistance of the boundaries. In this work, we propose a novel type of microflexible boundary condition for gradient-plasticity, which couples the slip transmission resistance with the phase-field damage such that the resistance locally changes during the fracturing process. The formulation allows maintaining the effect of grain boundaries as obstacles for plastic slip during plastification, while also accounting for weakening of their resistance during the softening phase. In numerical experiments, the new damage-dependent boundary condition is compared with classical microfree and microhard boundary conditions in polycrystals, and it is demonstrated that it indeed produces a response that transitions from microhard to microfree as the material fails. We show that the formulation maintains resistance to slip transmission during hardening, but can generate microcracks across grain boundaries during the fracture process. We further show examples of how the model can be used to simulate void coalescence and three-dimensional crack fronts in polycrystals.

1 | Introduction

Understanding the phenomena underlying ductile fracture is important for efficient design of many engineering components. Ductile fracture in metals usually occurs after significant plastic deformation. The fracture process proceeds from plastification to damage initiation, followed by the development of microscopic cracks and eventually the evolution of those into macroscopic cracks that can cause component failure. To simulate this process, it is important to develop models and computational

tools that are able to include the physical mechanisms on the grain scale.

Gradient-extended crystal plasticity models have for a long time been used to model size-dependent behavior of polycrystals see for example [1–4]. The size-dependence originates from geometrical necessary dislocations at grain boundaries and how they transmit as well as interact across interfaces like grain boundaries which influence crack initiation and propagation, compare for example [5]. In the context of gradient-extended crystal plasticity

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modeling, slip transmission mechanisms are accounted for by grain boundary conditions. Such conditions have been discussed in the literature for various gradient-extended plasticity models by introduction of interface energies, see for example [6, 7], or by accounting for slip direction mismatch and grain boundary orientation, see for example [8–12] and the review by Bayerschen et al. [13].

Damage initiates by void nucleation, often at inclusions and/or in shear bands. For ductile fracture, void nucleation frequently occurs inside single grains, even though it can occur at grain boundaries as well [14]. During the fracture process these voids grow and coalesce, whereby microcracks crossing grain boundaries are formed. The arrangement of voids as well as the way they coalesce strongly depends on the type of loading [15–17]. Damage and fracture within the grains may occur in the slip planes as a consequence of the localization of plastic slip. The propagation of microcracks follows crystallographic directions [18], whereby it is an appropriate choice to couple damage initiation with crystal plasticity on the grain scale, compare [19, 20].

While fracture of grains has in the past often been modeled by continuum damage combined with crystal plasticity models, for example [1, 19], phase-field methods have become a popular choice for modeling ductile fracture coupled to plasticity, see for example the overview of different ductile phase-field models by Alessi et al. [21] and references therein. One of the most advantageous features of phase-field modeling is that it allows arbitrary crack paths without suffering from a mesh dependence. Models coupling gradient plasticity and phase-field fracture have for example been suggested by Miehe, Aldakheel, and Raina [22] and, in a multi-physics context, been used by Kristensen, Niordson, and Martínez-Pañeda [23]. On the microscale, phase-field models have been coupled to various crystal plasticity models, compare for example [24–27]. We have recently suggested a thermodynamic modeling framework for finite strain gradient-enhanced crystal plasticity, which has so far been applied to single crystals [28].

The largest difference in terms of modeling polycrystals opposed to single crystals is the treatment of grain boundaries. Models combining gradient-extended plasticity and cohesive zone fracture at the grain boundaries of polycrystals have been suggested in for example [29] and [30]. Such models can be used to study the interplay between local stress concentrations at grain boundaries, which are influenced by the choice of grain boundary condition, and intergranular fracture. Spannraft et al. [31] have used a similar approach, but included an explicit coupling between the damage of cohesive element and the grain boundary condition. Specifically, the grain boundary condition that accounts for slip direction mismatch and grain boundary normal approaches a microfree condition as the damage of the cohesive element grows.

In this contribution, we base the model formulation on the framework presented in [28] for damage initiation and growth of microcracks in grains. The extension to the modeling of polycrystals in this paper requires a formulation of grain boundary conditions that should give size effects in the stress–strain response, but also allow for crack propagation across grain boundaries to yield realistic crack patterns. Therefore, we propose a novel thermodynamically consistent formulation of grain boundary conditions

with a coupling to the phase-field damage. The proposed coupling prescribes a damage dependent slip transfer resistance between the grains. The crystal plasticity phase-field fracture model from [28] is also extended by a volumetric-deviatoric split to account for the influence of stress triaxiality. Since both the gradient extended crystal plasticity and phase-field fracture model result in highly nonlinear problems and demand very fine spatial discretization, a grand challenge when simulating failure in polycrystals in 3D is the computational time. Therefore, we have formulated the gradient extension of the crystal plasticity to only act on a scalar measure whereby the size-dependence behavior still is captured while possible influence of slip direction mismatch is disregarded. This opens the way for feasible numerical studies of relations between microstructural characteristics and transgranular failure mechanisms observed in 3D polycrystals.

The paper is structured as follows: Section 2 first supplies a recapitulation of the thermodynamic modeling framework from [28] and subsequently proposed prototype model is described in Section 3. Section 4 introduces the field equations and the domains of the different fields with respect to the grain boundaries. It introduces different thermodynamically motivated choices of microboundary conditions, as well as the coupling between microflexible boundary conditions and the damage field. In Section 5 numerical experiments on polycrystals are presented and analyzed. The experiments yield insights into: the behavior of different choices of microboundary conditions upon damage development, the possibility to use the model for void coalescence predictions and its capability to produce three-dimensional crack fronts. Concluding remarks, as well as an outlook to possible future applications of the modeling framework are given in Section 6.

2 | Thermodynamic Framework

The model for gradient extended crystal plasticity and phase-field fracture of polycrystals is formulated within the thermodynamic framework presented in [28]. This section presents this framework in brief for completeness.

The multiplicative decomposition of the deformation gradient $\mathbf{F}$ into an elastic part $\mathbf{F}_e$ and a plastic part $\mathbf{F}_p$ is given by

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p \quad (1)$$

The free energy Ψ is assumed to depend on the elastic Cauchy-Green deformation gradient $\mathbf{C}_e = \mathbf{F}_e^T \cdot \mathbf{F}_e$, the set of isotropic hardening variables $\{k_\alpha\}_{\alpha=1}^{n_\alpha}$, where k_α is the isotropic hardening variable on the α -th of n_α slip systems, a damage (phase-field) variable d , the state variable q , and the set of spatial gradients $\{\nabla_0 k_\alpha\}_{\alpha=1}^{n_\alpha}$, as well as the spatial gradient $\nabla_0 d$, according to

$$\Psi = \Psi(\mathbf{C}_e, q, \{k_\alpha\}_{\alpha=1}^{n_\alpha}, \{\nabla_0 k_\alpha\}_{\alpha=1}^{n_\alpha}, d, \nabla_0 d) \quad (2)$$

The dissipation inequality when adopting quasi-static and isothermal conditions is given by

$$\int_{V_0} \mathbf{P} : \dot{\mathbf{F}} \, dV_0 - \int_{V_0} \dot{\Psi} \, dV_0 \geq 0 \quad (3)$$

where $\mathbf{P}$ is the first Piola-Kirchhoff stress and V_0 represents the initial domain with outer boundaries ∂V_0 . Subsequently, we also introduce the domains $V_{0,i}$, which refer to the grains of a polycrystal such that $V_{0,i}$ represents the i -th grain in a polycrystal with n_{grains} grains in total. Their respective grain boundaries are referred to as $\partial V_{0,i}$.

Using the standard Coleman-Noll arguments [32] the elastic second Piola-Kirchhoff stress $\mathbf{S}_e$ is obtained as (see e.g., [33]).

$$\mathbf{S}_e = 2 \frac{\partial \Psi}{\partial \mathbf{C}_e} \quad (4)$$

By introducing the Mandel stress $\mathbf{M}_e = \mathbf{C}_e \cdot \mathbf{S}_e$ and the plastic velocity gradient $\mathbf{L}_p = \dot{\mathbf{F}}_p \cdot \mathbf{F}_p^{-1}$, as well as using the divergence theorem, the dissipation inequality can be rewritten as

$$\begin{aligned} D = \int_{V_0} \left(\mathbf{M}_e : \mathbf{L}_p + Q \dot{q} + \sum_{\alpha=1}^{n_a} \kappa_{\alpha} \dot{k}_{\alpha} + Y_d \dot{d} \right) dV_0 \\ + \sum_{i=1}^{n_{\text{grains}}} \int_{\partial V_{0,i}} \sum_{\alpha=1}^{n_a} \kappa_{\alpha}^{\Gamma} \dot{k}_{\alpha} dA_0 + \int_{\partial V_0} Y_d^{\Gamma} \dot{d} dA_0 \geq 0 \end{aligned} \quad (5)$$

Therein, the following dissipative quantities were introduced

$$\kappa_{\alpha} = -\frac{\partial \Psi}{\partial k_{\alpha}} + \nabla_0 \cdot \frac{\partial \Psi}{\partial \nabla_0 k_{\alpha}}, \quad \kappa_{\alpha}^{\Gamma} = -\mathbf{N} \cdot \frac{\partial \Psi}{\partial \nabla_0 k_{\alpha}} \quad (6)$$

$$Y_d = -\frac{\partial \Psi}{\partial d} + \nabla_0 \cdot \frac{\partial \Psi}{\partial \nabla_0 d}, \quad Y_d^{\Gamma} = -\mathbf{N} \cdot \frac{\partial \Psi}{\partial \nabla_0 d} \quad (7)$$

$$Q = -\frac{\partial \Psi}{\partial q} \quad (8)$$

and $\mathbf{N}$ is the unit normal to the boundaries.

3 | Prototype Crystal Plasticity Model

In this section, we present a prototype gradient-extended crystal plasticity phase-field fracture model. We will assume the following form of the free energy, where a split of the elastic free energy contribution into a tensile part $\hat{\Psi}_e^+$ and a compressive part $\hat{\Psi}_e^-$ is adopted,

$$\begin{aligned} \Psi = g_e(d, \epsilon^p) \hat{\Psi}_e^+(C_e) + \hat{\Psi}_e^-(C_e) + \Psi_p(\{k_{\alpha}\}_{\alpha=1}^{n_a}, \{\nabla_0 k_{\alpha}\}_{\alpha=1}^{n_a}) \\ + \Psi_d(d, \nabla_0 d) \end{aligned} \quad (9)$$

Ψ_p and Ψ_d represent the free energy contributions associated with gradient crystal plasticity and phase-field fracture, respectively. Following, the three contributions to the free energy are defined.

3.1 | Hyper-Elasticity

The effective (undamaged) elastic part of the free energy $\hat{\Psi}_e$ is assumed to be of Saint-Venant type and a volumetric-deviatoric energy split is used, whereby the tensile and compressive parts of the elastic free energy are given by

$$\begin{aligned} \hat{\Psi}_e^+(E_e) = \frac{1}{2} K \langle \text{tr}(E_e) \rangle_+^2 + G E_e^{\text{dev}} : E_e^{\text{dev}} \quad \text{and} \\ \hat{\Psi}_e^-(E_e) = \frac{1}{2} K \langle \text{tr}(E_e) \rangle_-^2 \end{aligned} \quad (10)$$

where $E_e = (C_e - \mathbf{I})/2$ is the Green-Lagrange strain tensor and $\langle \bullet \rangle_{\pm} = (\bullet \pm |\bullet|)/2$ denotes the positive and negative parts of $\bullet$. K and G represent the bulk and shear modulus, respectively. The second Piola-Kirchhoff stress $\mathbf{S}_e$ is then derived from Equation (4) as

$$\mathbf{S}_e = g_e(d, \epsilon^p) 2 \frac{\partial \hat{\Psi}_e^+}{\partial C_e} + 2 \frac{\partial \hat{\Psi}_e^-}{\partial C_e} \quad (11)$$

Ductile failure is modeled using the elastic degradation function g_e presented by Ambati, Gerasimov, and De Lorenzis [34]

$$g_e(d, \epsilon^p) = (1 - d)^{2(\epsilon^p / \epsilon_{\text{crit}}^p)^n} \quad (12)$$

where ϵ^p is the accumulated plastic strain, which is represented by q in the thermodynamic modeling framework above. Notice that this formulation requires the development of plasticity as well as phase-field damage to degrade the material. This is expected behavior for ductile failure in metals and also leads to the recovery of a true elastic zone independently of the choice of surface energy functional. The critical accumulated plastic strain ϵ_{crit}^p and the exponent n determine how the development of plastic strain impacts the material degradation. As shown by [34], this degradation function formulation is thermodynamically consistent, that is $Q \dot{q} \geq 0$.

3.2 | Gradient-Enhanced Crystal Plasticity

The plastic free energy Ψ_p is chosen as

$$\Psi_p = \frac{1}{2} \sum_{\alpha=1}^{n_a} H_{\alpha} k_{\alpha}^2 + \frac{l_g^2}{2} \sum_{\alpha=1}^{n_a} \sum_{\beta=1}^{n_a} \nabla_0 k_{\alpha} \cdot \mathbf{H}_{\alpha\beta} \cdot \nabla_0 k_{\beta} \quad (13)$$

where the following material parameters were introduced: the isotropic hardening modulus H_{α} and the length scale for gradient-enhanced hardening l_g . Additionally, $\mathbf{H}_{\alpha\beta}$ determines gradient-enhanced cross-hardening between slip systems α and β . In general, the model allows to make distinct choices of $\mathbf{H}_{\alpha\beta}$ for gradient-enhanced self-hardening ($\alpha = \beta$) and gradient-enhanced cross-hardening ($\alpha \neq \beta$). However, in this work we choose $\mathbf{H}_{\alpha\beta} = H^g \mathbf{I}$ to be constant for all slip systems α, β . H^g can then be seen as gradient-enhanced hardening modulus. We adopt the standard assumption that the slip direction $\bar{s}_{\alpha}$ and normal vector to the slip plane $\bar{m}_{\alpha}$ on the intermediate configuration are fixed (and equal to their corresponding vectors on the undeformed configuration). The yield functions for the slip systems Φ_{α} are defined in terms of the effective Schmid stresses $\hat{\tau}_{\alpha}$

$$\Phi_{\alpha} = |\hat{\tau}_{\alpha}| - (\tau_y + \kappa_{\alpha}) \quad (14)$$

with $\hat{\tau}_{\alpha} = \tau_{\alpha} / g_e(d, \epsilon^p)$, wherein τ_{α} is the standard crystal plasticity Schmid stress $\tau_{\alpha} = \mathbf{M}_e^{\text{dev}} : (\bar{s}_{\alpha} \otimes \bar{m}_{\alpha})$. τ_y is the initial yield stress, which is the same for all slip systems here. We chose an associative evolution equation for the plastic velocity gradient

$$\begin{aligned} \bar{\mathbf{L}}_p = \dot{\mathbf{F}}_p \cdot \mathbf{F}_p^{-1} = \sum_{\alpha=1}^{n_a} \dot{\lambda}_{\alpha} \frac{\partial \Phi_{\alpha}}{\partial \mathbf{M}_e} \\ = \sum_{\alpha=1}^{n_a} \frac{\dot{\lambda}_{\alpha}}{g_e(d, \epsilon^p)} (\bar{s}_{\alpha} \otimes \bar{m}_{\alpha}) \text{sign}(\hat{\tau}_{\alpha}) \end{aligned} \quad (15)$$

and apply a viscoplastic regularization for the multiplier λ_α

$$\dot{\lambda}_\alpha = \frac{1}{t^*} \left\langle \frac{\Phi_\alpha}{\sigma_d} \right\rangle^m \quad (16)$$

where t^* , m and σ_d control the viscosity of the model and $\langle \bullet \rangle$ denotes Macauley brackets. The accumulated plastic strain ϵ^p is defined in terms of $\dot{\lambda}_\alpha$

$$\epsilon_p = \int_0^t \sqrt{\sum_{\alpha=1}^{n_a} \dot{\lambda}_\alpha^2} dt \quad (17)$$

The isotropic and gradient-extended hardening stresses κ_α and their boundary tractions κ_α^Γ , respectively, are derived from Equation (6) as

$$\kappa_\alpha = -H_\alpha k_\alpha + H_g^g l_g^2 \sum_{\beta=1}^{n_a} (\nabla_0 \cdot \nabla_0 k_\beta) \quad (18)$$

$$\kappa_\alpha^\Gamma = -H_g^g l_g^2 \mathbf{N} \cdot \sum_{\beta=1}^{n_a} \nabla_0 k_\beta \quad (19)$$

An associative evolution is assumed for the hardening strains k_α

$$\dot{k}_\alpha = \dot{\lambda}_\alpha \frac{\partial \Phi_\alpha}{\partial \kappa_\alpha} = -\dot{\lambda}_\alpha \quad (20)$$

These assumptions for the hardening can be extended, see for example, [35] to account for more complex models such as kinematic hardening, cross-hardening and nonlinear hardening.

3.3 | Phase-Field Fracture Model

An AT2 surface energy functional Γ_d (cf. [36]), is adopted for the phase-field model. The corresponding free energy contribution is given by

$$\Psi_d(d, \nabla_0 d) = \mathcal{G}_0^d \Gamma_d(d, \nabla_0 d) \quad \text{with} \quad \Gamma_d = \frac{1}{2\ell_0} (d^2 + \ell_0^2 |\nabla_0 d|^2) \quad (21)$$

where $\mathcal{G}_0^d$ represents critical fracture energy per unit area in the reference configuration and ℓ_0 is the length-scale parameter controlling the width of the diffuse crack model.

3.3.1 | Damage Irreversibility

Since phase-field models do not inherently possess damage irreversibility, it is necessary to incorporate a model extension to avoid damage healing upon unloading. One of the most common choices is the history variable approach [37]. It has, however, been shown to be variationally inconsistent. Within this work we instead use a micromorphic approach [38], which has recently been shown to allow for a variationally consistent framework that locally enforces damage irreversibility [39]. In [28], we showed how to combine the micromorphic irreversibility criterion with a gradient-enhanced crystal plasticity model and have demonstrated that this combination of models works well. In the micromorphic irreversibility formulation, an additional local variable φ is introduced, which represents the phase-field damage. The local phase-field damage φ and the

global phase-field damage d are then connected by a penalty term in the free energy, that is controlled by a penalty parameter α_p . All occurrences of d in the free energy, apart from that in the new penalty term and the gradient term $\nabla_0 d$, are then replaced by the new local damage variable φ .

$$\begin{aligned} \Psi = & g_e(\varphi, \epsilon^p) \hat{\Psi}_e^+(C_e) + \hat{\Psi}_e^-(C_e) + \Psi_p(\{k_\alpha\}_{\alpha=1}^{n_a}, \{\nabla_0 k_\alpha\}_{\alpha=1}^{n_a}) \\ & + \Psi_d(\varphi, \nabla_0 d) + \frac{\alpha_p}{2} (\varphi - d)^2 \end{aligned} \quad (22)$$

The dissipation inequality (5) is thereby modified to

$$\begin{aligned} D = & \int_{V_0} \left(\mathbf{M}_e : \mathbf{L}_p + Q \dot{q} + \sum_{\alpha=1}^{n_a} \kappa_\alpha \dot{k}_\alpha + Y_\varphi \dot{\varphi} + Y_d \dot{d} \right) dV_0 \\ & + \sum_{i=1}^{n_{\text{grains}}} \int_{\partial V_{0,i}} \sum_{\alpha=1}^{n_a} \kappa_\alpha^\Gamma \dot{k}_\alpha dA_0 + \int_{\partial V_0} Y^\Gamma d dA_0 \geq 0 \end{aligned} \quad (23)$$

where $Y_\varphi = -\partial\Psi/\partial\varphi$. Assuming that $Y_d = 0$ (Y_d energetic) yields the global phase-field equation

$$Y_d = \alpha_p (\varphi - d) + \mathcal{G}_0^d \ell_0 \nabla_0 \cdot \nabla_0 d = 0 \quad (24)$$

The penalty term introduces an additional regularization to the model. In [40] it was mainly used for numerical robustness, but here it is used to ensure damage irreversibility.

To exploit the micromorphic formulation for damage irreversibility, the evolution of the local phase-field φ is derived from the corresponding term of the dissipation inequality: $Y_\varphi \dot{\varphi} \geq 0$. For the proposed prototype model, $Y_\varphi = -\partial\Psi/\partial\varphi$ is obtained as

$$Y_\varphi = -\frac{\partial g_e}{\partial \varphi} \hat{\Psi}_e^+ - \frac{\mathcal{G}_0^d}{\ell_0} \varphi - \alpha_p (\varphi - d) \quad (25)$$

To ensure irreversibility of φ , an intermediate local variable is introduced with the property: $\tilde{\varphi} = \arg \{Y_\varphi(\varphi) = 0\}$. The Karush-Kuhn- Tucker conditions are then introduced to ensure irreversibility as follows:

$$\dot{\varphi} \geq 0, \quad \dot{\varphi} f_\varphi = 0, \quad f_\varphi = \tilde{\varphi} - \varphi \leq 0 \quad (26)$$

Thereby, we obtain $Y_\varphi \dot{\varphi} = 0$, since $Y_\varphi = 0$ during loading ($\varphi = \tilde{\varphi}$) and $\dot{\varphi} = 0$ during unloading ($\varphi = \text{const}$). Notice that the local phase-field here becomes a history variable. Thereby, thermodynamic consistency is fulfilled. Notice that the local phase-field φ also is a history variable in this formulation. The authors would also like to point out that the micromorphic phase-field irreversibility is a self-contained feature of the model formulation and can easily be exchanged for a more classical history variable irreversibility approach. In this case, the phase-field equation is still obtained from assuming that $Y_d = 0$, but Y_d is derived from Equation (9) instead of Equation (22).

4 | Weak Form of Balance Equations

We express the weak form of the equilibrium equation in terms of the first Piola-Kirchhoff stress $\mathbf{P}$ and neglect inertial forces as well as body forces

$$\begin{aligned} \delta \mathcal{W}^u = & \int_{V_0} \mathbf{P} : (\delta \mathbf{u} \otimes \nabla_0) dV_0 - \int_{\partial V_0} \mathbf{t}_0^* \cdot \delta \mathbf{u} dA_0 = 0 \\ & \forall \text{ kinem. admissible } \delta \mathbf{u} \end{aligned} \quad (27)$$

where t_0^* is a prescribed traction on the boundary ∂V_0 and the gradient of $\mathbf{u}$ and $\delta \mathbf{u}$ are square integrable. Since the expression for the gradient-extended hardening stress κ_α , Equation (6), includes spatial gradients, it also is a field equation. We adopt a dual mixed procedure [1], whereby a gradient hardening field $\mathbf{g}$ is defined as

$$\mathbf{g} = \sum_{\alpha=1}^{n_\alpha} \nabla_0 k_\alpha \quad (28)$$

The weak form of Equation (28) is then (instead of Equation (6)) introduced as a field equation and by using the divergence theorem we obtain the weak form for gradient (crystal) plasticity for all grains $i = \{1, \dots, n_{\text{grains}}\}$ as

$$\begin{aligned} \delta \mathcal{W}_i^g &= \int_{V_{0,i}} \mathbf{g} \cdot \delta \mathbf{g} \, dV_0 + \int_{V_{0,i}} \sum_{\alpha=1}^{n_\alpha} k_\alpha \nabla_0 \cdot \delta \mathbf{g} \, dV_0 \\ &\quad - \int_{\partial V_{0,i}} \sum_{\alpha=1}^{n_\alpha} k_\alpha \mathbf{N} \cdot \delta \mathbf{g} \, dA_0 = 0 \quad \forall \delta \mathbf{g} \end{aligned} \quad (29)$$

where the divergence of $\mathbf{g}$ and $\delta \mathbf{g}$ as well as k_α are square integrable. The gradient-extended hardening stress κ_α (Equation (18)) then becomes a local equation.

$$\kappa_\alpha = -H_\alpha k_\alpha + H^g l_g^2 \nabla_0 \cdot \mathbf{g} \quad (30)$$

This procedure has been shown to be numerically robust ([41, 42]). Additionally, it allows to easily exchange the underlying local crystal plasticity model, since such changes only affect local equations. Finally, the weak form of the global phase-field Equation (24) is given by

$$\begin{aligned} \delta \mathcal{W}^d &= \int_{V_0} \alpha_p (\varphi - d) \delta d \, dV_0 + \int_{\partial V_0} \mathcal{G}_0^d \ell_0 \mathbf{N} \cdot \nabla_0 d \delta d \, dA_0 \\ &\quad - \int_{V_0} \mathcal{G}_0^d \ell_0 \nabla_0 d \cdot \nabla_0 \delta d \, dV_0 = 0 \quad \forall \delta d \end{aligned} \quad (31)$$

where the standard boundary condition $\mathbf{N} \cdot \nabla_0 d = 0$ will be assumed on the outer boundary of the grain structure, such that the boundary integral term disappears. The gradient of d and δd as well as φ belong to the space of square integrable functions. The micromorphic penalty parameter should be chosen in relation to the effective fracture energy $\mathcal{G}_0^d / \ell_0$, for example using a dimensionless scalar β and choosing $\alpha = \beta \mathcal{G}_0^d / \ell_0$.

Equations (27), (29) and (31) are to be solved for polycrystals, which requires the definition of how the respective fields should behave at grain boundaries. Since this work is concerned with transgranular fracture, the displacement field $\mathbf{u}$ is assumed to be continuous across grain boundaries. The gradient field $\mathbf{g}$ on the other hand is a measure for the dislocation distribution and since grain boundaries restrict the dislocation movement in polycrystals, the gradient field $\mathbf{g}$ is in general discontinuous. While dislocation transport across grain boundaries can occur in reality, we here make the simplification that the gradient field $\mathbf{g}$ is independent in each grain. The damage field d is assumed to be continuous across grain boundaries.

4.1 | Microflexible Boundary Conditions

Requirements on the boundary conditions for the strain gradient field $\mathbf{g}$ follow from thermodynamic consistency. For the chosen prototype model, the boundary term relating to gradient (crystal) plasticity in the reduced dissipation inequality, Equation (5), is given by

$$\begin{aligned} &\sum_{i=1}^{n_{\text{grains}}} \int_{\partial V_{0,i}} \sum_{\alpha=1}^{n_\alpha} (\kappa_\alpha^\Gamma \dot{k}_\alpha) \, dA_0 \\ &= \sum_{i=1}^{n_{\text{grains}}} \int_{\partial V_{0,i}} \left(-H^g l_g^2 \mathbf{N} \cdot \mathbf{g} \right) \sum_{\alpha=1}^{n_\alpha} \dot{k}_\alpha \, dA_0 \geq 0 \end{aligned} \quad (32)$$

This is a stronger requirement than postulated by Equation (5), however we will prove that the proposed boundary conditions can satisfy this requirement and thereby also satisfy Equation (5). There are two trivial ways to fulfill the inequality in Equation (32):

1. Microfree boundary conditions: $\kappa_\alpha^\Gamma = 0$, corresponding to Dirichlet-type constraints by prescribing $\mathbf{N} \cdot \mathbf{g} = 0$ in the dual-mixed formulation.
2. Microhard boundary conditions: $\sum_{\alpha=1}^{n_\alpha} k_\alpha = 0$ and thereby $\dot{k}_\alpha = 0$. This corresponds to removing the boundary integral in the weak form for gradient plasticity, Equation (29).

Additionally to these two classical types of boundary conditions, we propose microflexible boundary conditions inspired by the formulation in [8]. We prescribe the sum of hardening strains on the boundary such that

$$\sum_{\alpha=1}^{n_\alpha} k_\alpha = C_\Gamma \kappa^\Gamma \quad (33)$$

where a microflexibility parameter C_Γ has been introduced and

$$\kappa^\Gamma = \kappa_\alpha^\Gamma = -H^g l_g^2 \mathbf{N} \cdot \mathbf{g} \quad (34)$$

since κ_α^Γ for the proposed model is the same for all slip systems. The boundary dissipation in Equation (32) thereby becomes

$$\sum_{i=1}^{n_{\text{grains}}} \int_{\partial V_{0,i}} \frac{1}{C_\Gamma} \sum_{\alpha=1}^{n_\alpha} k_\alpha \sum_{\alpha=1}^{n_\alpha} \dot{k}_\alpha \, dA_0 \geq 0 \quad (35)$$

Therein, all signs are known: From the evolution equations, Equation (20), we know that $\dot{k}_\alpha \leq 0$ and with an initial value of $k_\alpha^{\text{initial}} = 0$, it follows that $k_\alpha \leq 0$. Thus, by choosing $C_\Gamma > 0$ thermodynamic consistency of the boundary term is guaranteed. Upon applying microflexible boundary conditions the weak form for gradient plasticity, Equation (29) becomes

$$\begin{aligned} \delta \mathcal{W}_i^g &= \int_{V_{0,i}} \mathbf{g} \cdot \delta \mathbf{g} \, dV_0 + \int_{V_{0,i}} \sum_{\alpha=1}^{n_\alpha} k_\alpha \nabla_0 \cdot \delta \mathbf{g} \, dV_0 \\ &\quad + \int_{\partial V_{0,i}} \left(C_\Gamma H^g l_g^2 \mathbf{N} \cdot \mathbf{g} \right) (\mathbf{N} \cdot \delta \mathbf{g}) \, dA_0 \\ &\quad \forall i = \{1, \dots, n_{\text{grains}}\} \end{aligned} \quad (36)$$

The boundary term therein can be implemented as a standard boundary integral (over all grain boundaries) in the finite element framework, as it only includes constants, the normal vector to the boundary $\mathbf{N}$ and the field variable $\mathbf{g}$. Note that for $C_\Gamma \rightarrow 0$ microhard boundary conditions are recovered. Microfree boundary conditions are recovered when $C_\Gamma \rightarrow \infty$, since in this case $\kappa^\Gamma \rightarrow 0$ is required for satisfying the residual equation. Grain boundaries present obstacles for the propagation of plastic slip, thereby causing a grain size dependent stress-strain response in polycrystals, also known as the Hall-Petch effect. The resistance to plastic slip across a grain boundary depends, for example, on the misorientation angle between the slip systems of the grains meeting at the boundary and their accumulated plastic slip. See formulations for this in for example [8, 9], and [10]. Varying resistance to plastic slip from grain boundary to grain boundary can be accounted for by adjusting the (initial) value of the microflexibility parameter C_Γ . However, the dependence of the misorientation angles between single slip systems is for simplicity disregarded in this work to focus on transgranular fracture and the interaction with slip transmission resistance as well as to obtain feasible computational times. To account for the effect of fracture on the resistance of grain boundaries to plastic slip, we propose to couple the microflexibility parameter C_Γ with the phase-field damage d such that an increased d lowers the resistance. In this way a boundary can evolve from being initially microhard to a microfree boundary. The presented modeling framework allows for other choices of influence of the damage on the microflexibility. For the presented prototype model, a linear relation between the microflexibility and the phase-field damage is chosen according to

$$C_\Gamma(d) = C_{\Gamma,0} + C_\Gamma^d d \quad (37)$$

where $C_{\Gamma,0}$ is the initial microflexibility of each grain boundary and C_Γ^d represents the additional amount of microflexibility gained by complete material degradation. The microflexibility parametrization should always be chosen relative to the gradient hardening parameters. By this choice of C_Γ , the finite element problem, Equation (36), and the $\mathbf{g}$ -field become uncoupled between the grains (apart from an implicit coupling via $\mathbf{u}$ and d).

5 | Numerical Experiments

The behavior of the proposed model is discussed with respect to different aspects of damage initiation in this section. First, examples of the base cases of microfree and microhard boundary conditions are shown to discuss the qualities and flaws of both choices. It is then demonstrated how microflexible boundary conditions coupled to the damage development combine the desirable features of those boundary conditions. Finally, we show that the model is able to capture relevant phenomena in (ductile) fracture such as void coalescence and three-dimensional crack fronts.

Figure 1 shows the two different grain structures that are used for the numerical examples. The two-dimensional examples are performed on a structure consisting of 10 grains and using plane strain conditions. The same grain structure is first investigated without the voids shown in Figure 1 and then with the voids. The three-dimensional examples are performed on a structure consisting of 4 grains. In all cases full FCC slip systems are used for all grains. The used meshes contain mesh refinements along the grain boundaries and at grain boundary intersections. The two-dimensional meshes consist of 22 616 (without voids) and 45 688 (with voids) linear triangular elements, respectively. The three-dimensional mesh consists of 76 506 linear tetrahedral elements. Further details of the geometries and their meshing are given in Appendix B. All structures are loaded in-plane by displacement-controlled pure shear loading. As introduced in Section 4, two vector fields (displacement field $\mathbf{u}$ and gradient field $\mathbf{g}$) and a scalar field (global phase-field damage d) are needed on each node. While the displacement field $\mathbf{u}$ and the phase-field d are continuous fields, the gradient field $\mathbf{g}$ is independent in each grain. This is achieved by duplicating the nodes on the grain boundaries and then applying linear constraints on the grain boundaries for the displacement field $\mathbf{u}$ and the phase-field d , which allows to use the same mesh representation for all fields. Backward Euler time integration is applied to all time-dependent equations, see Appendix C for the respective derivations. A staggered solver is used to solve the coupled equation system. The initial time step is $\Delta t_{\text{initial}} = 0.1 t^*$, the time

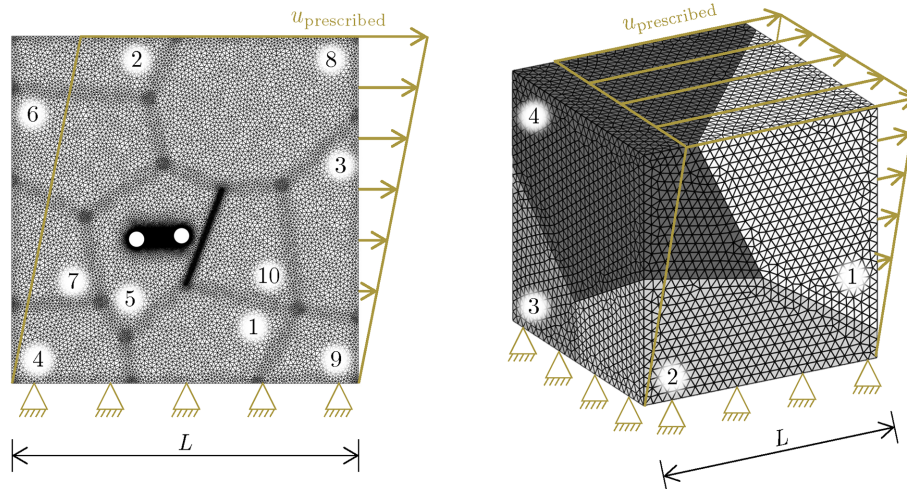


FIGURE 1 | Two- (left) and three-dimensional (right) grain structures used for the numerical experiments. The two-dimensional structure consists of 10 grains and is used with and without the voids in the middle grain. Without voids, the middle grain is meshed in the same manner as the other grains. The three-dimensional grain structure consists of four grains. All set-ups are loaded by simple shear along the horizontal axis.

step is halved whenever a load step does not converge. For an iterative solver to succeed on this type of phase-field problems, it is important that the staggered scheme extends to the local variables. Further, methods for avoiding unneeded iterations far away from the solution are used. A detailed description of the solver algorithm and its respective parameters, is given in Appendix D. This work focuses on model development rather than model parametrization, for details on material parameters, slip system orientations and loading, consult Appendix A.

The implementation of the presented model is written in the Julia programming language [43] and uses the Ferrite.jl finite element toolbox [44]. The material model implementation

makes heavy use of the Tensors.jl tensor calculus toolbox [45], that supports automatic differentiation of tensor equations, and all figures are generated by the Makie.jl data visualization ecosystem [46].

5.1 | Impact of Boundary Conditions for Gradient Plasticity

Microfree and microhard boundary conditions

Figures 2 and 3 show the bounding cases of microfree and microhard boundary conditions on the inner grain boundaries.

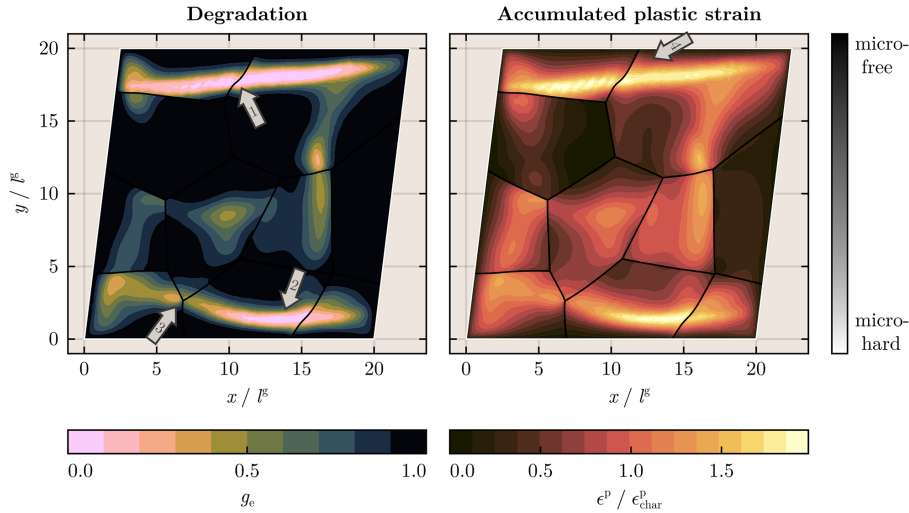


FIGURE 2 | Degradation and plastic strain response for **microfree boundary conditions** on the inner grain boundaries. Both fully developed cracks cross grain boundaries. Localization of plastic strain initially occurs in the grain marked with arrow 1, close to the grain boundary. The bottom crack (arrow 2) develops later in the simulation. Its crack growth direction is impacted by the stress concentration caused by the grain boundary intersection marked with arrow 3. The microfree boundary conditions are reflected by the accumulated plastic strain contour lines that are perpendicular to the grain boundaries, especially in the highly plastified regions (e.g., arrow 4). Microhard boundary conditions are prescribed on the outer boundaries of the grain structure for numerical stability.

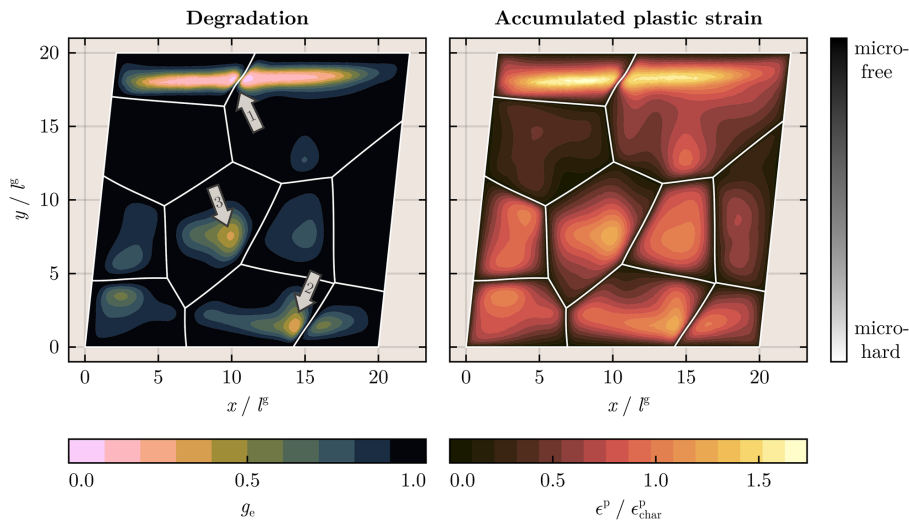


FIGURE 3 | Degradation and plastic strain response for **microhard boundary conditions** on the inner grain boundaries. The crack developing within the upper grains is interrupted on the grain boundary marked by arrow 1. Localization of plastic strain initially occurs inside the grain right of that grain boundary. Plastic strain cannot develop on the grain boundaries. Microhard boundary conditions are prescribed on the outer boundaries of the grain structure.

Note that microhard boundary conditions are used for the outer boundaries in all simulations to stabilize the global response for the Newton-Raphson solver. To the left of both figures, the degradation g_e is presented, displaying the cracks formed at the end of the simulation. To the right, the corresponding accumulated plastic strain ϵ^p distribution, normalized by the characteristic accumulated plastic strain ϵ_{char}^p is shown. In both figures, the grain boundaries are colored in gray scale where dark means microfree and light means microhard boundary conditions. In particular, the black-to-white colorscale represents $C_r = C_{r,0} = 1/\left(H^g l_g^2\right)$ as microhard and $C_r = 9/\left(H^g l_g^2\right)$ as microfree; however, note that the microfree limit is chosen based on the contour plots for the accumulated plastic strain ϵ^p and used exclusively for post-processing purposes.

The accumulated plastic strain is an important input to the degradation function, as well as a representative quantity for the hardening variables k_α . Microfree boundary conditions require that the component of the gradient hardening field $\mathbf{g}$ perpendicular to the grain boundaries is zero. In Figure 2, this is reflected by contour lines of ϵ^p which are perpendicular to the boundaries, especially on those grain boundaries where a large amount of plastic strain has developed (e.g., pointed out by arrow 4). Notice however, that $\mathbf{g} = \sum_{\alpha=1}^{n_a} \nabla_0 k_\alpha$ is only fulfilled in a weak sense. Microfree boundary conditions allow the development of plastic strain on the grain boundaries. Initial strain localization is to a large extent influenced by the alignment of crystal orientations with the loading direction, as well as by geometrical features. Initial localization sites are often located at grain boundaries or grain boundary intersections. The upper crack for example initiates on the right side of the grain boundary marked by arrow 1. Later in the simulation a second crack develops, which initiates in the grain marked by arrow 2. The growth direction of the secondary crack is strongly influenced by the stress concentration occurring at the grain boundary intersection marked by arrow 3. Microhard boundary conditions on the other hand require that $\sum_{\alpha=1}^{n_a} k_\alpha = 0$ on the boundary, in a weak sense. This is reflected in Figure 3 by contour lines of ϵ^p which are parallel to the grain boundaries. In particular, microhard boundary conditions disallow the development of plastic strain on the grain boundaries. This is important in combination with the choice of degradation function, see Equation (12), since it also results in disallowing damage development on the grain boundaries. Consequently, the first crack in Figure 3 (arrow 1), is interrupted by the respective grain boundary. The microhard simulation shows two damage initiation sites in addition to the developed crack, which are marked with arrows 2 and 3 in Figure 3. Comparing with the crack pattern arising from the microfree simulation, it can be observed that both simulations develop a similar primary crack. The precise shape of the crack is impacted by the choice of microfree/microhard boundary conditions. Additionally, the damage initiation site marked by arrow 2 in the microhard results corresponds to the damage initiation site of the secondary crack in the microfree results (compare Figure 2). Thus, the presented model predicts that the boundary conditions on gradient hardening have a significant impact on the crack growth across grain boundaries, but not on the damage initiation sites.

Both cases, microfree and microhard boundary conditions, exhibit physically partly correct and partly incorrect behavior for

the representation of ductile fracture in polycrystalline metals. Grain boundaries represent obstacles for dislocation movement. This is represented by microhard boundary conditions, causing an elastic response close to the grain boundaries (plastic deformation is caused by dislocation movement, thus preventing dislocation movement leads to an elastic response). This is also how the size-dependent stress-strain response in polycrystals is captured by gradient-plasticity models. Additionally, damage initiation commonly occurs inside the grains and not on the grain boundaries as implied by the microfree results shown in Figure 2. However, the resistance of a given grain boundary to dislocation movement depends among other things on the misalignment between the slip system orientations on both sides of the boundary. Grain boundaries also do not present ultimate obstacles for crack growth, as implied by the microhard results shown in Figure 3.

Microflexible boundary conditions

To address the lack of accuracy of the microfree and microhard boundary conditions in describing the full range from strain localization to damage initialization and finally fracture, we use the microflexible boundary condition presented in Section 4.1. Under the assumption that the resistance of grain boundaries against dislocation movement decreases as damage develops, we suggest that the initial behavior of grain boundaries can be approximated by microhard boundary conditions while the behavior close to material failure should be approximated by microfree boundary conditions. As described in Section 4.1, this is implemented by assigning a low initial microflexibility $C_{r,0}$ (low microflexibility recovers microhard behavior) that gradually increases as the global damage field d increases (high microflexibility recovers microfree behavior). Figure 4 displays the resulting fracture and plasticity patterns. It can be seen that the obtained cracks each span several grains and pass the grain boundaries in a similar manner as for the microfree case. By inspecting the white-to-black color scale on the grain boundaries, it can be noticed that the grain boundaries locally transition from microhard to microfree behavior. It can be observed that most grain boundaries remain closer to the microhard state, while the boundary conditions locally change to microfree at the locations where the material is most degraded. Arrow 3 marks a grain where the remaining microhard boundary conditions can be noticed particularly well from the contour lines of the accumulated plastic strain. Similarly to the microfree case, the upper crack (arrow 1) develops first and the lower crack (arrow 2) develops later. The latter crack is also impacted by the same stress concentration as in the microfree simulation.

Additionally, strain and damage localization are distinctly observable in Figure 4. The grain boundary marked by arrow 1 exhibits a clear s-shaped deformation, as well as a clear local transition to microfree boundary conditions. This displays the need for a finite strain formulation, as well as the effect of the localized effect of microflexible boundary conditions.

Figure 5 shows the volume-averaged shear component of the second Piola-Kirchhoff stress in the upper two grains (where the first crack develops in all simulations). It shows that the microhard boundary conditions lead to a stiffer response than the microfree boundary conditions. Microflexible boundary conditions behave

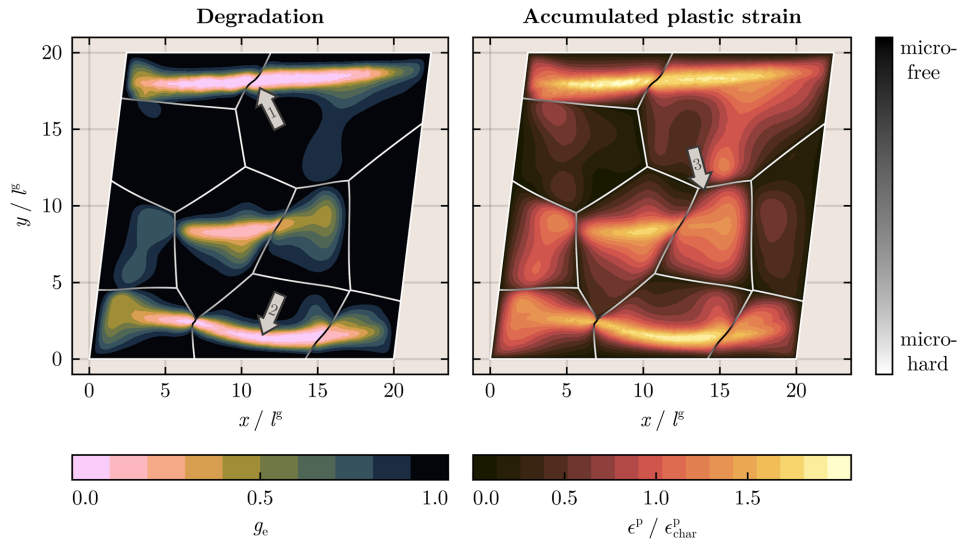


FIGURE 4 | Degradation and plastic strain response for **microflexible boundary conditions** on the inner grain boundaries. The damage initiation side of the upper crack is indicated by arrow 1. The crack initiates on the right side of the grain boundary and then propagates to the left grain. The microflexible boundary conditions initially behave nearly microhard and upon damage development locally transition to microfree behavior. The state of the microboundary conditions at the end of the simulation is color-coded on a white to black color scale in the figure. Microhard boundary conditions are prescribed on the outer boundaries of the grain structure for numerical stability.

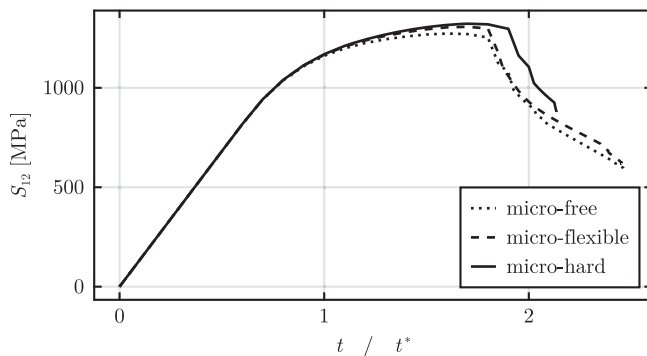


FIGURE 5 | Volume averaged in-plane shear component of the second Piola-Kirchhoff stress tensor in the upper two grains, comparing different inner microboundary conditions. Microhard boundary conditions lead to a stiffer response than microfree boundary conditions. As desired, microflexible boundary conditions initially behave similarly to microhard boundary conditions and then approach the behavior of microfree boundary conditions during the softening period.

similarly to microhard boundary conditions during the hardening stage, but similarly to microfree boundary conditions during the softening stage. Thus, they recover the physically meaningful behavior over the full plastification and fracture range.

5.2 | Void Coalescence

Crack initiation often occurs due to void nucleation and growth. Voids commonly nucleate on particles and inclusions placed within shear bands. The following example shows damage growth from preexisting voids in a grain structure. The voids are here modeled as holes in the structure and microfree boundary conditions are used at the void boundaries. The voids are positioned in the middle crack shown in Figure 4. This is the last

crack that develops in the microflexible simulation. The resulting crack pattern is shown in Figure 6. The developed crack pattern is different from the one obtained in Figure 4. The cracks indicated by arrows 1 and 2 develop simultaneously, where the crack developing between the voids (arrow 1) is clearly more developed than the crack in the top grains (arrow 2). Due to the crystal plasticity model the susceptibility of the grains to plasticity and thereby damage initiation highly depends on the crystal orientation of each grain relative to the loading direction. The multi-axial stress state caused by the voids leads to the activation of slip systems that were not triggered in the previous examples and thereby causes the failure marked by arrow 1. This crack has a crack shielding effect, which prevents the development of the bottom crack compared with the original microflexible simulation.

5.3 | Three-Dimensional Crack Fronts

Crack fronts in polycrystals are strongly influenced by the grain structure, crystal orientations and the misalignment thereof, as well as voids and particles in the metal matrix. Hence, these crack fronts inherently propagate in three-dimensional space and it is not always possible to understand their behavior from two-dimensional simulations. The presented modeling framework is formulated in a dimension-agnostic manner and can thereby account for such three-dimensional effects. The final numerical example shows the response of a three-dimensional four-grained polycrystal to in-plane shear loading. To allow for a coarser mesh, the length scale parameters have been adjusted to $l_g = 0.1333 L$ and $l_0 = 0.08 L$. The microflexibility parameters, as well as the micromorphic penalty parameter are adjusted accordingly, see Table A1.

Figure 7 shows the resulting degradation and accumulated plastic strain fields. To better represent the crack fronts, all degradation values $g_e \leq 0.17$ are represented as transparent. Simple shear

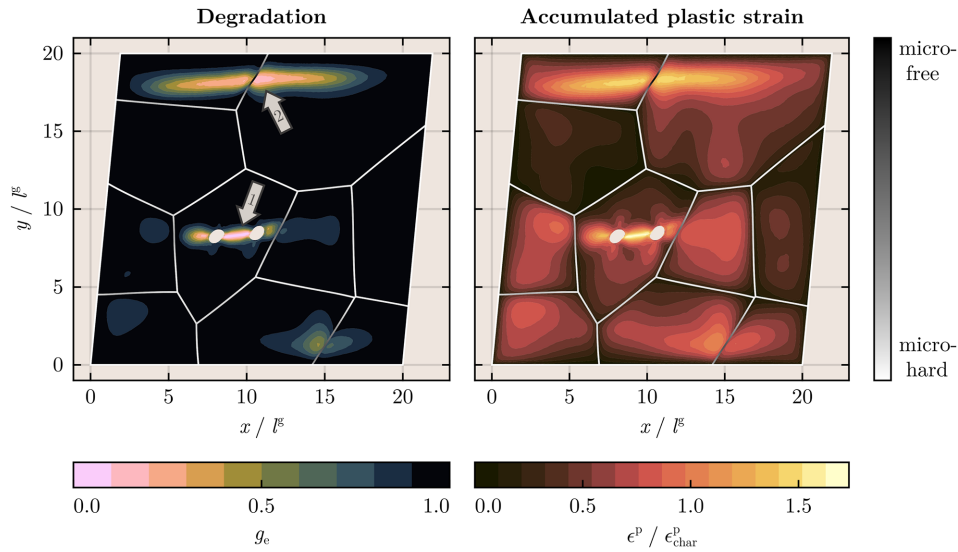


FIGURE 6 | Degradation and plastic strain response for a case of void coalescence with **microflexible boundary conditions** on the inner grain boundaries. Preformed voids perturb the fracture pattern compared with Figure 4 and lead to an additional crack, caused by void coalescence inside the middle grain (arrow 1). The multi-axial stress state around the voids activates slip systems that are otherwise not triggered by the global loading and thereby causes the failure of the originally undamaged grain. Microhard boundary conditions are prescribed on the outer boundaries of the grain structure for numerical stability.

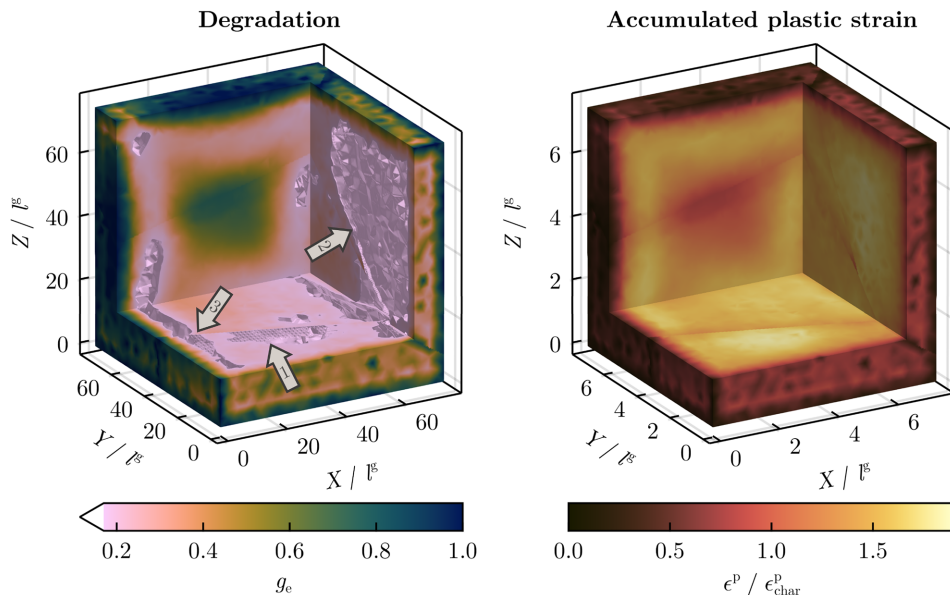


FIGURE 7 | Degradation and plastic strain response for the four-grain three-dimensional grain structure. **Microflexible boundary conditions** are prescribed on the inner grain boundaries, while microhard boundary conditions are prescribed on the outer boundaries of the grain structure for numerical stability. In the degradation plot all regions with degradation values $g_e \leq 0.17$ are represented as transparent to better visualize the resulting crack fronts. The structure is oriented as presented in Figure 1 and thus shear is applied in the XZ-plane. Several crack fronts have developed. It can be observed that the crack fronts on the right and in the middle of the grain do not range along the entire Y-axis and could therefore not be captured by a plane strain set-up.

is applied in the XZ-plane, with roller supports along the front and back faces in the Figure. Notice that opposed to the previous two-dimensional results, the three-dimensional results are presented in the initial configuration. The larger length scales for gradient plasticity and phase-field damage lead to wider shear bands and cracks. The final state of the simulation shows a complex crack front that has developed in the structure. The visualization in Figure 7 shows a cut into part of the crack front.

It can be observed that parts of the crack front do not range all the way along the Y-axis (marked by arrows 1 and 2), indicating that they could not have been resolved by a 2D plane strain simulation. This can in particular be observed at the right part of the crack front (arrow 2), which developed within grain 1 and does not cross the boundary to grain 4 (arrow 2 points on the grain boundary). The crack front developing on the left (arrow 3) on the other hand displays the impact of the microflexible boundary

conditions. It reaches across the grain boundary between grain 2 and grain 3, the point where it crosses the grain boundary is marked by arrow 3.

6 | Concluding Remarks

In this work, we have presented a modeling framework and a prototype model for ductile phase-field fracture across grain boundaries of polycrystals. The model fits a thermodynamic framework, that we have presented in previous work [28] in the context of single crystal plasticity.

The prototype model presented in our previous work has been extended to account for properties of polycrystals. In particular, we have presented a damage-dependent microflexible boundary condition that allows for modeling of grain boundaries that exhibit varying slip transmission resistance. The level of resistance is tunable by a microflexibility parameter, which we use to locally vary boundary conditions from microhard to microfree upon damage development. The presented boundary condition is represented by a standard boundary integral including field variables and material parameters. Hence, it is straightforward to implement it in a finite element setting. Further, we have added a volumetric-deviatoric energy split to the prototype model to allow a physically reasonable difference in fracture behavior of tension and compression. This is relevant for polycrystals, since the microstress state caused by the grain structure can easily yield local compression even under shear loading. It is also important for obtaining realistic behavior upon crack closure.

We have moreover used a single gradient hardening field in the dual mixed formulation, instead of one gradient field per slip system as presented in [28]. This represents a significant reduction in the computational effort required for solving the problem (especially in 3D) and allows to consistently work with the full set of 12 FCC slip systems. Numerical examples show that damage-dependent microflexible boundary conditions are, opposed to simpler microfree and microhard boundary conditions, able to capture a realistic hardening response as well as crack development and propagation across grain boundaries. It is also shown that the model can be used to simulate coalescence of pre-existing voids. Furthermore, fracture of polycrystals is inherently a three-dimensional problem and although the necessary mechanisms can be comprehensively demonstrated on two-dimensional examples, crack fronts develop differently in three-dimensional grain structures. We show that our model is able to produce three-dimensional crack fronts by applying it to a three-dimensional polycrystal.

The presented modeling framework opens up for future investigation of damage initiation and microcrack formation under consideration of the influence of grain boundary behavior. The role of grain boundaries as obstacles for the transport of plastic slip and how to model varying degrees of resistance against slip transmission has been a central topic of the presented work. We have used the simplification that grain boundaries act as slip sinks. In reality, however, the process of slip transmission from one grain to the other is much more complex and depends among other things on the misalignment of crystal orientations and the type of dislocations. To account for the process of

(partial) slip transmission between the grains on each side of the grain boundary, it is possible to extend the model by methods that allow to account for jumps in the field equations such as cohesive elements. To capture the plastic slip resistance of each slip system based on misalignment angles, the microflexible boundary condition could be derived for a model that accounts for the plastic slip gradient in each slip system separately, such as the one presented in [28]. The authors want to point out that such models, especially in combination with complex per-slip system boundary conditions come at a largely increased computation cost, as well as a significantly larger set of parameters.

Finally, the presented model is built to capture damage initiation and formation of microcracks. An important mechanism during damage initiation is void nucleation, which often occurs at hard particles. Upon combining this work with a contact model, it should be possible to simulate void nucleation by debonding at hard particles, as for example observed by Achouri et al. [47] and different localization patterns during void nucleation as discussed by Noell, Carroll, and Boyce [16]. To simulate void coalescence leading up to component failure, it is often necessary to develop solvers that can trace unstable crack growth, such as arc-length solvers. Recently, dissipation based arc-length solvers have shown good performance for phase-field models and seem to be a promising approach for thermodynamically consistent models such as the one presented in this work [48, 49].

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Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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Appendix A

Material Parameters

Material parameters for the two-dimensional simulations are given in Table A1. The length scales for the three-dimensional simulation deviate such that $l_g = 0.1333 L$ and $\ell_0 = 0.08 L$. The other parameters are adjusted as presented in Table A1. All simulations use full FCC

slip-systems, see Table A2 for the unit cell slip systems. To account for the different crystal orientations in the grains, the unit cell of each grain is rotated according to the Rodrigues parameters given in Table A3.

The loading rate at the upper side of the structures is $0.05 L / t^*$. The sides are loaded accordingly, to achieve displacement controlled simple shear loading conditions.

TABLE A1 | Base material parameters used for the numerical experiments. L is a global length scale for the simulated structure and results are independent of L upon scaling. Size independence of the model can be derived in the same way as demonstrated in [28].

Parameter		Value	Unit
Bulk modulus	κ	71660	MPa
Shear modulus	μ	27260	MPa
Yield stress	τ^y	345	MPa
Isotropic hardening modulus	H_{iso}	250	MPa
Gradient hardening modulus	H^g	1000	MPa
Gradient hardening length scale	l_g	$0.0533 L$	
Viscoplastic relaxation time	t^*	1	s
Viscoplastic drag stress	σ^d	500	MPa
Viscoplastic exponent	m	8	—
Initial microflexibility	$C_{\Gamma,0}$	$1 / (H^g l_g^2)$	
Microflexibility slope	C_{Γ}^d	$20 / (H^g l_g^2)$	
Effective fracture energy	$\mathcal{G}_0^d / \ell_0$	300	N/mm ²
Phase-field length scale	ℓ_0	$0.02 L$	
Micromorphic penalty parameter	α	$200 \mathcal{G}_0^d / \ell_0$	
Critical plastic strain	ϵ_{crit}^p	0.1	—
Degradation exponent	n	2	—

TABLE A2 | FCC slip systems. The unit cell of each grain in the numerical examples is rotated as described in Table A3.

α	$\bar{s}_\alpha$	$\bar{m}_\alpha$	α	$\bar{s}_\alpha$	$\bar{m}_\alpha$	α	$\bar{s}_\alpha$	$\bar{m}_\alpha$	α	$\bar{s}_\alpha$	$\bar{m}_\alpha$
1	$\begin{bmatrix} \bar{1} & 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$	4	$\begin{bmatrix} \bar{1} & \bar{1} & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & \bar{1} & \bar{1} \end{bmatrix}$	7	$\begin{bmatrix} 1 & 1 & 0 \end{bmatrix}$	$\begin{bmatrix} \bar{1} & 1 & \bar{1} \end{bmatrix}$	10	$\begin{bmatrix} 1 & \bar{1} & 0 \end{bmatrix}$	$\begin{bmatrix} \bar{1} & \bar{1} & 1 \end{bmatrix}$
2	$\begin{bmatrix} 1 & 0 & \bar{1} \end{bmatrix}$	$\begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$	5	$\begin{bmatrix} 1 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & \bar{1} & \bar{1} \end{bmatrix}$	8	$\begin{bmatrix} \bar{1} & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} \bar{1} & 1 & \bar{1} \end{bmatrix}$	11	$\begin{bmatrix} \bar{1} & 0 & \bar{1} \end{bmatrix}$	$\begin{bmatrix} \bar{1} & \bar{1} & 1 \end{bmatrix}$
3	$\begin{bmatrix} 0 & \bar{1} & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$	6	$\begin{bmatrix} 0 & 1 & \bar{1} \end{bmatrix}$	$\begin{bmatrix} 1 & \bar{1} & \bar{1} \end{bmatrix}$	9	$\begin{bmatrix} 0 & \bar{1} & \bar{1} \end{bmatrix}$	$\begin{bmatrix} \bar{1} & 1 & \bar{1} \end{bmatrix}$	12	$\begin{bmatrix} 0 & 1 & 1 \end{bmatrix}$	$\begin{bmatrix} \bar{1} & \bar{1} & 1 \end{bmatrix}$

TABLE A3 | Rodrigues angles for the rotation of the FCC unit cell in each grain. The left table shows the angles for the 2D grain structure with 6 grains, the right table shows the angles for the 3D grain structure with 4 grains.

Grain	2D Rodrigues angles				Grain	2D Rodrigues angles			
1	−3.67	2.54	−0.52		6	1.12	−1.05	−1.1	
2	3.8	22.4	16.75		7	1.4	2.07	−0.64	
3	−6.32	5.63	−27.73		8	0.55	−0.53	−0.55	
4	−0.22	0.26	−0.1		9	0.71	−0.94	1.02	
5	0.08	0.54	0.02		10	−0.97	−0.42	0.37	

Grain	3D Rodrigues angles			
1		0.70		1.81
2		−1.76		1.73
3		2.56		−1.54
4		−0.35		0.09

Appendix B

Geometry and Meshing Details

The polycrystals are generated by the open-source software Neper [50]. The prompts for generating the two- and three-dimensional tessellations are `neper-T-dim 2-n 10-id 2` and `neper-T-dim 3-n 4-id 1`, respectively. The voids in the two-dimensional structure are placed at positions $[0.36 L, 0.415 L]$ and $[0.49 L, 0.425 L]$ and have a diameter of $0.045 L$. All meshes are generated by `gmsh` [51]. The average element sizes in the different areas of the meshes are given in Table B1.

TABLE B1 | Mesh characteristics: Average element sizes in the different areas of the meshes and number of nodes/elements.

Element size	2D polycrystal	2D polycrystal with voids	3D polycrystal
Background mesh	$0.0125 L$	$0.0125 L$	$0.053333 L$
Grain boundaries	$0.00875 L$	$0.00875 L$	$0.040000 L$
Grain boundary intersections	$0.005 L$	$0.005 L$	$0.040000 L$
Voids	—	$0.0005625 L$	—
Between voids	—	$0.001125 L$	—
Grain boundary right of voids	—	$0.00225 L$	—
Number of nodes	12 146	24 033	16 065
Number of Triangles/Tetrahedra	22 616	45 688	76 506

Appendix C

Time Integration

By applying backward Euler time integration to Equations (15) and (20) and discretizing Equations (17) and (26), time-discretized forms of the local variables are obtained

$${}^{n+1}\mathbf{F}_p^{-1} = {}^n\mathbf{F}_p^{-1} \cdot \left(\mathbf{I} - \sum_{\alpha=1}^{n_\alpha} \frac{{}^{n+1}\Delta\lambda_\alpha}{{}^{n+1}g_e({}^{n+1}\varphi, {}^{n+1}\epsilon^p)} (\bar{\mathbf{s}}_\alpha \otimes \bar{\mathbf{m}}_\alpha) \right) \text{sign}({}^{n+1}\tau_\alpha) \quad (\text{C1})$$

$${}^{n+1}k_\alpha = {}^nk_\alpha - {}^{n+1}\Delta\lambda_\alpha \quad (\text{C2})$$

$${}^{n+1}\epsilon^p = {}^n\epsilon^p + \sqrt{\sum_{\alpha=1}^{n_\alpha} {}^{n+1}\Delta\lambda_\alpha^2} \quad (\text{C3})$$

$${}^{n+1}\varphi = \max({}^n\varphi, {}^{n+1}\varphi^{\text{trial}}) \quad (\text{C4})$$

The signs of the Schmid stresses ${}^{n+1}\tau_\alpha$ can be computed based on elastic trial stresses. Since all local variables can then be expressed in terms of ${}^{n+1}\Delta\lambda_\alpha$ and ${}^{n+1}\varphi^{\text{trial}}$, it remains to solve the coupled equation system resulting from Equations (16) and (25)

$$\begin{aligned} &\mathcal{R}_{\Delta\lambda_\alpha}({}^{n+1}\Delta\lambda_\alpha, {}^{n+1}\varphi^{\text{trial}}) \\ &= {}^{n+1}\Delta\lambda_\alpha - \frac{\Delta t}{t^*} \left\langle \frac{\Phi_\alpha({}^{n+1}\Delta\lambda_\alpha, {}^{n+1}\varphi^{\text{trial}})}{\sigma_d} \right\rangle^m = 0 \end{aligned} \quad (\text{C5})$$

$$\begin{aligned} &\mathcal{R}_{\varphi^{\text{trial}}}({}^{n+1}\Delta\lambda_\alpha, {}^{n+1}\varphi^{\text{trial}}) \\ &= -\frac{\partial g_e({}^{n+1}\varphi^{\text{trial}}, {}^{n+1}\Delta\lambda_\alpha)}{\partial \varphi} \hat{\Psi}_e^+ - \frac{G_0^d}{\ell_0} {}^{n+1}\varphi^{\text{trial}} \\ &- \alpha ({}^{n+1}\varphi^{\text{trial}} - d) = 0 \end{aligned} \quad (\text{C6})$$

Notice that while $\mathcal{R}_{\Delta\lambda_\alpha}$ implicitly depends on ${}^{n+1}\varphi^{\text{trial}}$ via Equation (C4), $\mathcal{R}_{\varphi^{\text{trial}}}$ explicitly depends on it, meaning it solves $\mathcal{Y}_\varphi(\varphi^{\text{trial}}) = 0$.

Appendix D

Staggered Solver

A staggered solver is used to solve the coupled equation system. Equations (27) and (29) are solved in a monolithic way in the first step, referred to by $\mathcal{R}^{\text{ug}}$ in Figure D1, Equation (31) is solved in the second step, referred to by $\mathcal{R}^d$, in each staggered iteration. We apply field-wise tolerances and each field can converge either based on a tolerance on its residual equation (residual tolerance) or on the update of the variable vector within a single Newton iteration (field tolerance). The solver algorithm is represented in Figure D1. In the same manner as presented in [28], the staggered scheme extends to the local level. Therefore, the global fields $\mathbf{u}$, $\mathbf{g}$ and d , as well as the local variables $\Delta\lambda_\alpha$ and φ^{trial} are split into two sets. Set 1 includes $\{\mathbf{u}, \mathbf{g}, \Delta\lambda_\alpha\}$, which are the variables relating to $\mathcal{R}^{\text{ug}}$ and Set 2 includes $\{d, \varphi^{\text{trial}}\}$, relating to $\mathcal{R}^d$. In each step only the set of variables relating to the solved equations can be updated, while the other set of variables is frozen to the values of the previous iteration. Since the two local variables are part of different sets, this means that each local residual equation is solved separately and only in one of the two staggered steps.

In each staggered step, the global and local residual equations are solved by Newton iterations. After solving the system corresponding to the respective staggered step, convergence of the global residual equation corresponding to the other staggered step is checked. If both global residual equations fulfill the convergence criteria without further updates of the variables, the time step is converged.

The convergence criteria for the global residual equations are given in Table D1. The iterations on the local residual equation use a fixed tolerance of 10^{-8} . To cut unnecessary iterations when solving each of the global residual equations, coarser back-up tolerances can be used (early) in the field iterations. However, the use of the back-up tolerances always triggers further iterations between the fields and thus a time step can never finally converge based on the back-up tolerances. The use of the back-up tolerances can be triggered by any of the following scenarios:

- The residual tolerance is still larger than the back-up tolerance in a set iteration `iter_backuptol`.
- Either of the previous two solves (one on each step) has used more than `n_iter_backuptols` iterations AND the first computed residual is larger than the back-up tolerance. `n_iter_backuptols` is chosen for each step separately.
- The maximum number of iterations `max_iter` is reached, but the final tolerances are not fulfilled.

These solver parameters are given in Table D2. Additionally, iterations are terminated when divergence is recognized as follows:

- Field iterations: The first residual in a solve is larger than the first residual of the previous solve more than `max_field_divergence` times in a row (for the same residual equation).
- Newton iterations for each solve: The residual has increased more than `max_divergence_count` subsequent times.

Within the Newton iterations, a basic line search is applied. Upon increasing residuals, the computed variable update $\Delta\mathbf{a}$ is reduced such that $\Delta\mathbf{a} = 0.7^{\text{number of increases}} \Delta\mathbf{a}_{\text{original}}$.

When a time step fails (e.g., due to recognized divergence or lack of material model convergence), the time step is halved. Time step halving is allowed up to `max_time_refinement_level` times. After `n_timesteps_recoarsen` converged time steps in a row, the time step is doubled if the previous time step did not use more than `n_field_iter_coarsen` field iterations. Time step doubling is not allowed to lead to coarser time steps than the initial time step $\Delta t_{\text{initial}}$.

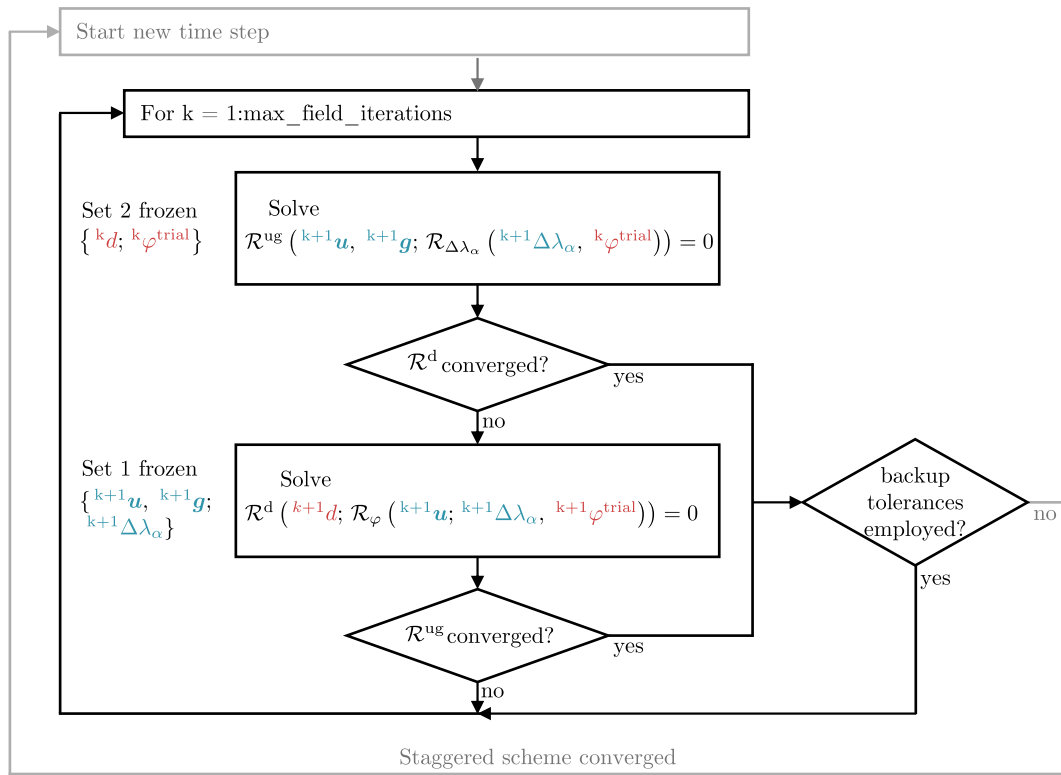


FIGURE D1 | Staggered solver: The residual equations are solved in two steps, where the first step ($\mathcal{R}^{\text{ug}}$) consists of the equilibrium equation and the gradient plasticity equation and the second step consists of the phase-field equation ($\mathcal{R}^{\text{d}}$). Iterations between the two steps go back and forth until all global residual equations fulfill the final convergence criterion for the same global variables. During the iteration process, unnecessary iterations are cut by allowing each single step to converge according to back-up tolerances. However, convergence according to the back-up tolerances does not allow to leave the field iteration loop.

TABLE D1 | Field-wise tolerances applied for global convergence examination. A field is considered converged when either of the residual or the field tolerance (Relating to the update of field variables during a single Newton-correction) is fulfilled. L is assumed to have unit mm.

		Weak form	Residual tolerance	Field tolerance
Final tolerances	Displacement field $\mathbf{u}$	Equation (27)	$L^2 \cdot 10^{-6} \text{ Nmm}^{-2}$	$L \cdot 10^{-8}$
	Hardening strain gradient $\mathbf{g}$	Equation (29)	$L^2 \cdot 10^{-11}$	$L^{-1} \cdot 10^{-6}$
	Global phase-field d	Equation (31)	$L^3 \cdot 10^{-10} \text{ Nmm}^{-3}$	10^{-8}
Back-up tolerances	Displacement field $\mathbf{u}$	Equation (27)	$L^2 \cdot 10^{-3} \text{ Nmm}^{-2}$	$L \cdot 10^{-8}$
	Hardening strain gradient $\mathbf{g}$	Equation (29)	$L^2 \cdot 10^{-8}$	$L^{-1} \cdot 10^{-6}$
	Global phase-field d	Equation (31)	$L^3 \cdot 10^{-10} \text{ Nmm}^{-3}$	10^{-8}

TABLE D2 | Parameters used in the staggered solver.

Solver parameter	value
max_field_iter	500
max_iter	25
iter_backuptol	8
n_iter_backuptols for $\mathcal{R}^{\text{ug}}$	25
n_iter_backuptols for $\mathcal{R}^{\text{d}}$	2
max_field_div	2
max_divergence_count	5
max_time_refinement_level	20
n_field_iter_coarsen	20