Modeling of Single-Slip Finite Strain Crystal Plasticity via the Virtual Element Method

Christoph Böhm[1,*], **Blaž Hudobivnik**[1], **Fadi Aldakheel**[1], and **Peter Wriggers**[1]

[1] Institute of Continuum Mechanics, Leibniz University Hanover, An der Universität 1, 30823 Garbsen, Germany

This work addresses an efficient low order virtual element method (VEM) for the modeling of single-slip crystal plasticity system undergoing finite deformations. VEM has been attracting attention as a novel scheme within the field of computational mechanics. A key advantage of VEM is the ability of constructing an arbitrary element shapes that can be non-convex [1]. Another important aspect is that VEM fits the grain shapes of crystal plasticity within polycrystalline aggregates *perfectly*. Contrary, classical finite element (FE) approaches request a fine mesh-size at possibly sharp geometric regions, i.e. complex shaped grain boundaries.

1 Introduction

During the last decade, the request for locally adapted material response, induced by lightweight strategies, was undergoing a constant increase. The collaborative research centre 1153 (CRC 1153) investigates the production of hybrid workpieces, showing such response. The physical effects, exhibiting at the joining zone of hybrid structures, are located at the microscopic length scale. In the micro-mechanics of polycrystalline materials, i.e. metals, the plasticity is affected by the underlying crystal lattice structure. Such microstructural environments exhibit highly heterogeneous geometric properties such like grain shapes, possibly non-convex, as well as rotations of the particular grains. In literature, studies address widely the mechanics of materials, modeled within the framework of virtual elements, i.e. thermo-elasto-plastic coupled behavior in [2, 3], forming processes in [4] or fracture analysis in [5, 6]. However, by addressing a crystal plasticity formulation at polycrystalline aggregates, the VE-performance remains still an open question. This work aims to bridge this gap by providing a finite strain crystal plasticity model, embedded within a virtual element framework at a heterogeneous microstructure.

2 Constitutive Framework and Computational Approach

The microstructure is modeled using the principle of representative volume element ($\mathcal{RVE}$), introduced at grain-level of the polycrystalline aggregate. The rotation of the grains is captured by a set of pseudo-random generated angles $\varphi_i \in [0,\ 2\pi]$ with $i \in \{1,\ 2,\ 3\}$, denoting particular Euler-rotations. The response of each grain g is described by an incremental work potential [7]:

$$\psi_g = \psi_{lat,g} + \psi_h + \delta t \psi_{dis}, \quad \psi_{lat,g} = \psi_{iso} + \psi_{ani,g}, \quad \psi_{ani,g} = c \sum_{i=1}^{3} (K_i - 1)^2, \tag{1}$$

where $\psi_{lat,g}$ denotes the stored elastic energy due to the lattice, splitted into an isotropic contribution ψ_{iso}, covered by a standard Neo-Hookean model, and a lattice structure specific contribution. The anisotropy is governed by invariants $K_i = \mathrm{Tr}(\mathbf{C}_e \mathbf{M}_i)$, with $\mathbf{M}_i = \mathbf{a}_i \otimes \mathbf{a}_i$ being the structural tensor of the i-th preferred direction. The hardening due to movements of dislocations through the lattice is modeled with a linear hardening ansatz by an introduction of the energy function $\psi_h = \frac{1}{2}\gamma^2 h_0$. Herein, c and h_0 are particular material parameters. Following [7], the plastic slip contribution of the work potential is modeled by an incremental dissipation function $\delta t \psi_{dis}$, with $\delta t = t - t_n$ being the time-increment. The computation of the results is reached by the minimization of a potential:

$$U := \sum_g \int_{\mathcal{G}_g} \psi_g \mathrm{d}\mathcal{RVE} - \mathcal{P}_{ext}(\mathbf{u}), \tag{2}$$

where $\mathcal{P}_{ext}$ denotes the potential, induced by external loads. The virtual element method is based on a split of the primary fields $\mathcal{R}$ into a projected part and a remainder, introduced in [1], to:

$$\mathcal{R}_h = \Pi\mathcal{R}_h + (\mathcal{R}_h - \Pi\mathcal{R}_h), \quad \Pi\mathcal{R}_h = \sum_{i=1}^{3} (N_\Pi \cdot \mathbf{a}_i)\, \mathbf{e}_i, \quad N_\Pi = \{1, X, Y, Z\}, \tag{3}$$

* Corresponding author: e-mail boehm@ikm.uni-hannover.de, phone +49 511.762-2285, fax +49 511.762-5496

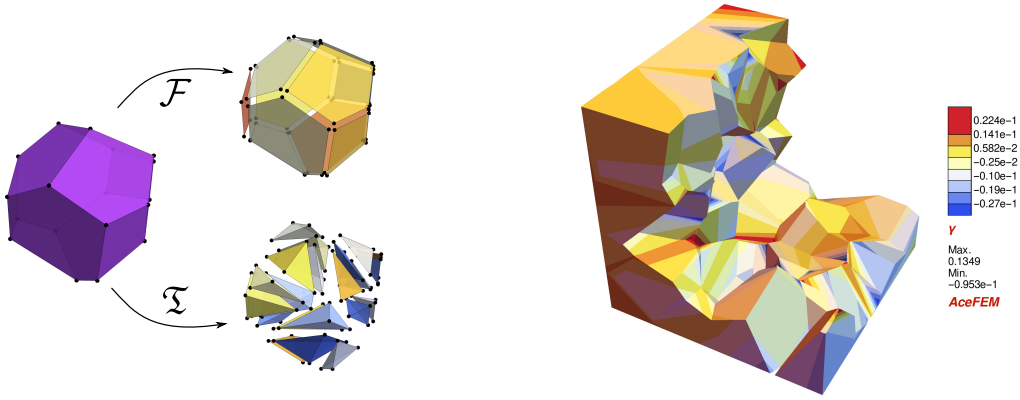
with Π denoting the projection operator that projects the virtual space to its polynomial space of order one. A linear ansatz, illustrated in [2], for the projected primary fields $\Pi\mathcal{R}_h$ is used. N_Π is a vector, collecting a constant 1 and the spatial coordinate variables, belonging to the basis vectors $\mathbf{e}_i$ with $i \in \{1, 2, 3\}$. Hence, $\mathbf{a}_i = \{a_{i1}, ..., a_{i4}\}$ are the coefficients, defining $\Pi\mathcal{R}_h$ in each element $\mathcal{G}$. Following [8], the potential U is undergoing a decomposition into a consistency and a stabilization terms:

$$U(\nabla\mathcal{R}_h, \mathcal{R}_h) = \mathop{\mathbf{A}}_{\mathcal{G}}\Big[(1-\beta)U(\nabla\Pi\mathcal{R}_h|_{\mathcal{G}}, \Pi\mathcal{R}_h|_{\mathcal{G}}) - \beta U(\nabla\mathcal{R}_h|_{\mathcal{G}}, \mathcal{R}_h|_{\mathcal{G}})\Big], \tag{4}$$

with $\beta \in [0, 1]$ being a fraction to control the stabilization influence and being computed by following the ansatz in [1]. The element residual and the element tangent matrix are computed by utilizing automatic differentiation based tools within the software ACEGEN/ACEFEM [9], which is a subpackage of MATHEMATICA.

3 Representative Numerical Example

The projection is computed by utilizing a decomposition of the virtual element $\mathcal{G}$ into its faces $\mathcal{F} \in \partial\mathcal{G}$. Whereas its stabilization term is computed on a triangulated submesh of tetrahedron $\mathfrak{T} \in \mathcal{G}$, see **Fig. 1**a).



a) b)

Fig. 1: a) Schematic illustration of the decomposition of a polyhedral virtual element $\mathcal{G}$ into its faces $\mathcal{F}$ and its internal mesh, consiting of tetrahedral elements $\mathfrak{T}$; b) Plot of shear γ, acting on the plane $(1\ 1\ 1)$ of a fcc lattice structure, resulting from an uniaxial tension test $\mathbf{u} = \mathbf{E}\mathbf{x}$ with fixed stabilization $\beta = 0.4$.

The resulting plastic shear γ of an uniaxial tension test within $\mathbf{e}_1$ direction, by applying constant strain $\mathbf{E}_{ij} = 1$ with $i, j = 1$ for $\mathbf{u} = \mathbf{E}\mathbf{x}$ is illustrated in **Fig. 1**b). The influence of the anisotropic lattice structure as well as its pseudo-random rotations are observed on the plastic shear γ. Furthermore, Fig. 1b) demonstrates the development of the plasticity through the particular grains within the $\mathcal{RVE}$.

Acknowledgement

CB, FA and PW gratefully acknowledge the German Research Foundation (DFG, Deutsche Forschungsgemeinschaft) for the financial support to this work with the Collaborative Research Centre 1153 (CRC 1153) "*Process chain for the production of hybrid high-performance components through tailored forming*" with the subproject C4 "*Modelling and Simulation of the Joining Zone*", project number 252662854.

References

[1] B. Hudobivnik, F. Aldakheel, and P. Wriggers, Computational Mechanics **63**(2), 253–269 (2019).
[2] F. Aldakheel, B. Hudobivnik, and P. Wriggers, International Journal for Multiscale Computational Engineering **17**(2) (2019).
[3] F. Aldakheel, B. Hudobivnik, and P. Wriggers, Computational Mechanics **64**(5), 1347–1360 (2019).
[4] C. Böhm, J. Kruse, M. Stonis, F. Aldakheel, and P. Wriggers, Procedia Manufacturing **47**, 713–718 (2020).
[5] F. Aldakheel, B. Hudobivnik, A. Hussein, and P. Wriggers, Computer Methods in Applied Mechanics and Engineering **341**, 443–466 (2018).
[6] A. Hussein, F. Aldakheel, B. Hudobivnik, P. Wriggers, P. A. Guidault, and O. Allix, Finite elements in analysis and design **159**, 15–32 (2019).
[7] C. Miehe, S. Mauthe, and F. Hildebrand, Computer Methods in Applied Mechanics and Engineering **268**, 735–762 (2014).
[8] M. Cihan, F. Aldakheel, B. Hudobivnik, and P. Wriggers, arXiv preprint arXiv:2002.02680 (2020).
[9] J. Korelc and P. Wriggers, Automation of Finite Element Methods (Springer, 2016).