## THE HIGHER-DIMENSIONAL CONTINUUM DISLOCATION DYNAMICS BASED PLASTICITY APPROACH WITH APPLICATION TO A THIN FILM TENSION TEST

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In this paper we consider the numerical approximation of an elasto-plastic micro-structure model based on the evolution of dislocations using the higher-dimensional Continuum Dislocation Dynamics (hdCDD) theory. For this purpose we introduce a coupling of a Runge-Kutta discontinuous Galerkin (RKDG) method for the dislocation model with a finite element method (FEM) handling the occuring stress fields from the macro-structure due to the elastic boundary value problem (BVP).

The hdCDD theory [1, 2] describes the evolution of curved dislocation lines based on a higher-dimensional description of discrete dislocations. Systematic averaging of discrete dislocation configurations leads to a representation through continuum field equations for a higher-dimensional dislocation density tensor. First numerical results were realized in [3] using finite difference methods.

We will introduce a reformulation of an evolution system of this theory in conservative form,  $\partial_t \mathbf{u} + \nabla \cdot \mathbf{F}(\mathbf{u}, v) = \mathbf{f}(\mathbf{u}, v)$ , where  $\mathbf{u} := (\rho, q)$  and  $\rho, q, v : \Gamma \times S^1 \to \mathbb{R}$  are the dislocation density, the curvature density and the scalar velocity of dislocations, respectively; here  $\Gamma \subset \mathbb{R}^2$  is a crystallographic slip plane and  $S^1 = \mathbb{R}/(2\pi \mathbf{Z})$ . This formulation allows to use a discontinuous Galerkin (DG) method for the spatial discretization together with an explicit Runge-Kutta method as time integrator.

We define the discretization of the elastic problem using FEM such that the faces of the elements can also serve as mesh for the hdCDD slip planes. Hence, we only have one common mesh for the elastic BVP and all slip planes. This setup also is anvantageous for parallel computation due to an easy mesh distribution and a communication of the coupled system.

We introduce a new element for the DG method that uses tensor products of Fourier functions and polynomials as basis functions to reduce the higher-dimensionality of hdCDD. As numerical example, we perform a tension test as in [4] with one active slip system as illustrated in Figure 1. Dirichlet boundary conditions are used on top and bottom of the elastic body and free boundaries are used over each hdCDD slip plane. As a result of the tension test, we obtain the stress-strain curve as in Figure 2. It can be devided into three different regimes and accounts for changing hardening behavior due to the flux of dislocations (Fig.2). The numerical results are realized with the parallel finite element system M++ [5].



Figure 1: Sketch of slip planes embedded into the elastic domain



Figure 2: Stress - strain curve: (I) elastic regime  $(E = m_1)$ , (II) plastic regime induced by loop expansion  $(E = m_2$  is reduced), (III) starvation due to outflux of edge dislocations and remaining screw dislocations  $(E \approx 2m_2)$ 

## REFERENCES

- T. Hochrainer, M. Zaiser, P. Gumbsch : A three-dimensional continuum theory of dislocations : kinematics and mean field formulation. *Philosophical Magazine*, 87 (2007), 1261–1282.
- [2] T. Hochrainer, S. Sandfeld, M. Zaiser, P. Gumbsch : Continuum dislocation dynamics: Towards a physical theory of crystal plasticity. J. Mech. Phys. Solids, (2013).
- [3] S. Sandfeld, T. Hochrainer, P. Gumbsch, M. Zaiser : Numerical implementation of a 3D continuum theory of dislocation dynamics and application to micro-bending. *Philosophical Magazine*, 90 (2010), 3697–3728.
- [4] Z.L. Liu, Z. Zhuang, X.M. Liu, X.C. Zhao, Z.H. Zhang : A dislocation dynamics based higher-order crystal plasticity model and applications on confined thin-film plasticity. *International Journal of Plasticity*, 27 (2011), 201–216.
- [5] C. Wieners : A geometric data structure for parallel finite elements and the application to multigrid methods with block smoothing. *Comp. Vis. Sci.*, 13 (2010), 161–175.