Numerical Implementation and Application of a Three-Dimensional Continuum Theory of Curved Dislocations

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In recent years, the growing demand for physically motivated continuum theories of plasticity has led to a renewed effort to formulate continuum theories of dislocation kinematics and dynamics.

In the late 1950s, Kröner, Nye, Bilby and Kondo independently formulated the classical continuum theory of dislocations based upon the definition of a dislocation density tensor ('Kröner-Nye tensor'). The authors were well aware that this tensor, if used as a measure of the average dislocation state of a crystal, leads to a description of plastic deformation processes that is intrinsically incomplete. In particular, the Kröner-Nye tensor is only a measure for the geometrically necessary dislocations while all information about statistically stored dislocations is lost at larger scales. As a consequence, any spatially homogeneous shear deformation can in principle not be reflected by the dynamic evolution of the Kröner-Nye tensor or similar measures. This renders the classical dislocation density measure highly problematic as a foundation for a continuum theory of plasticity.

Many shortcomings of the classical theory were recently remedied by the introduction of an extended continuum theory of curved dislocations developed at IZBS in cooperation with M. Zaiser, University of Edinburgh (cf. Dissertation Hochrainer, 2006). This theory utilizes a generalisation of the Kröner-Nye tensor, the so-called dislocation density tensor of second order. Within this tensor all dislocations are considered as line-like objects. This was achieved by the so-called 'lift' of curves: a map of the spatial curve into a higher-order configuration space. When considering only one slip system, the configuration space consists of the spatial slip plane *x-y* and the dislocation line orientation φ. In this configuration space an extended dislocation density tensor $\boldsymbol{\alpha}^{II}$ is defined as a differential form. This tensor is defined by the scalar dislocation density ρ giving the density of dislocations with orientation φ and the mean dislocation curvature *k:*

$$\alpha^{II} = \rho\left(cos\varphi dy \wedge d\varphi - sin\varphi dx \wedge d\varphi + k dx \wedge dy\right) \otimes b$$

The temporal change of $\boldsymbol{\alpha}^{II}$ is governed by a conservation law, which can be converted into evolution equations for the scalar dislocation density ρ and for the mean curvature k.

In this project we study the extended continuum theory for the quasi-two-dimensional case of a single glide system. To numerically validate the theory we show that the continuum evolution equation of this new dislocation density measure can handle the kinematic evolution of quasi-discrete dislocation loops. Furthermore, the case of homogeneous loop distribution can be easily treated numerically within this theory. This is a simple case where theories which rely on the Kröner-Nye tensor, normally fail.

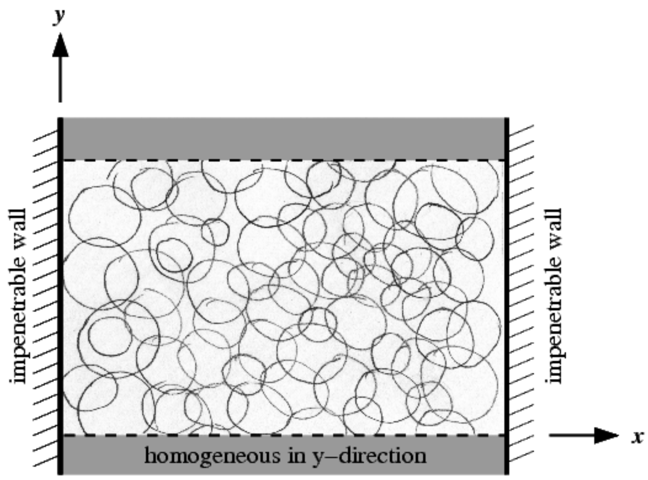

Fig. 1: Sketch of a distribution of dislocation loops in a constrained slip channel. We consider a one-dimensional special case where the movement of dislocations is hindered by impenetrable walls at the left and the right side of the geometry, while assuming an infinitely long and homogeneous distribution in y-direction. Close to the walls line orientations parallel to the walls dominate the distribution

The numerical application aims at predicting the dislocation evolution and mechanical behaviour of realistic systems like a conductor line used in a micro chip. Towards this goal we modelled impenetrable boundary conditions with the extended continuum theory. This was achieved by prescribing a velocity function and evolving a curvature field k as well as a density field ρ, both of which are defined in the configuration space (Fig. 1).

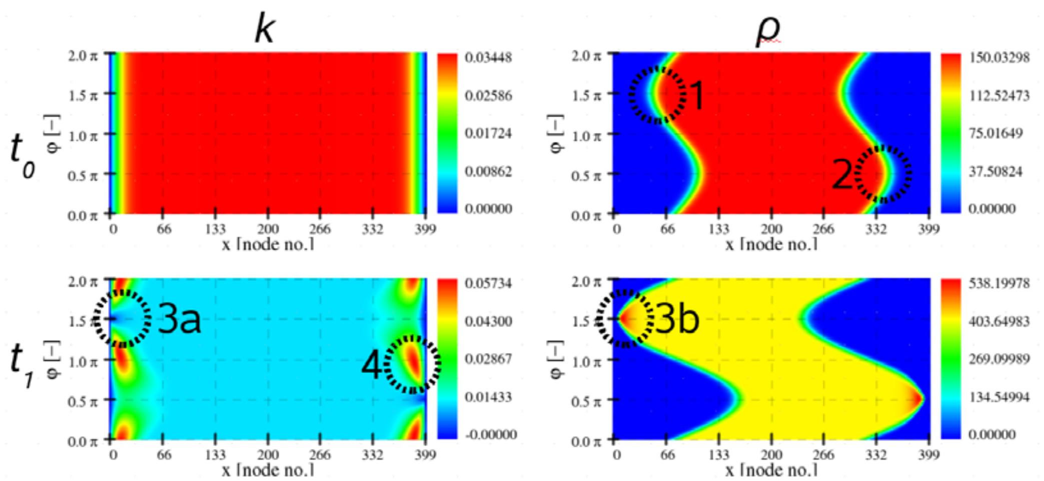

Fig. 2: Evolution of average dislocation curvature k (left) and dislocation density (right) in a constrained channel geometry. The horizontal axis shows the channel width, the vertical axis is the dislocation line orientation φ, the y axis is omitted since k and ρ are constant in this direction. **Top row:** Initial loop curvature (left) and density (right) at time t_0.=0. The curvature is mostly constant, which implies that the initial system is a distribution of circular loops. The markings '1' and '2' represent the density corresponding to a line orientation parallel to the left and right interface, respectively. **Bottom row**: Evolved curvature and density field at time $t_1>t_0$. The markings '3a' and '3b' denote the point where dislocations have zero curvature parallel to the channel wall (i.e. corresponds to a straight line segment) and a high density gets disposed at the interface. The area '4' is the intermediate region where the deposited line segments bow out (with a large curvature) back into circular shape (=constant curvature in the field area).