Leaving the Slip System - Cross Slip in Continuum Dislocation Dynamics

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Dislocations are the main contributors to plastic deformation of crystalline materials. An important step towards the description of hardening behavior is the consideration of cross slip, as it drives the exchange of dislocations between slip systems, thus playing a major role in dislocation multiplication or annihilation.

In density based continuum theories of dislocations, dislocations are usually considered closed curves within their slip planes. Recent discrete dislocation dynamics simulations, however, suggest that only a small fraction of dislocations is actually closed on a single slip system, due to cross slip and dislocation reactions. We therefore investigate how the kinematics of moving open curves can be considered in dislocation density based models.

The assumption of open planar curves leads to modified evolution equations for the dislocation state variables. These extended evolution equations are presented for the theory of geometrically necessary dislocations (GND) and for the higher dimensional continuum dislocation dynamics theory (hdCDD). The resulting equations are checked for plausibility by numerical calculations using the finite volume method.

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1 Kinematics of Open Curves in GND theory

In the GND theory, the main quantity describing the state of the system is the dislocation density tensor $\alpha$, which can be obtained as the curl of the plastic distortion tensor. It can also be defined slip system wise as the tensor product of the dislocation density vector $\rho^s$ with the burgers vector $b^s$

$$\alpha = \sum_s \alpha^s = \sum_s \rho^s \otimes b^s.$$  \hspace{1cm} (1)

The constraint $\text{div} \rho^s = 0$ ensures that the dislocations are closed lines on each slip system. For further information about the GND theory, the reader is referred to [1].

The kinematic description of the system is given by an evolution equation for this density measure. For closed curves, the evolution equation is known as Mura’s equation

$$\partial_t \alpha^s = \text{curl} (v^s \times \alpha^s),$$ \hspace{1cm} (2)

where $v^s$ is the average dislocation velocity. The velocity is assumed to be perpendicular to the line direction contained in $\rho^s$. In the following, the slip system index $s$ will be dropped, but all equations are understood for one specific slip system.

Since the burgers vector is constant within each slip system, it can be omitted from equation (2), yielding an analogous evolution equation for the dislocation density vector $\rho$.

The kinematics of a density of open dislocations can be obtained by dropping the zero divergence assumption. Using a Lie derivative, the evolution equation for $\rho$ is found as

$$\partial_t \rho = \text{curl} (v \times \rho) - v_b \text{div} \rho,$$ \hspace{1cm} (3)

where $v_b$ is the average boundary point velocity. Note that $v_b$ is not necessarily perpendicular to the line direction. Figure 1 shows the evolution of a dislocation density mimicking a single open loop. The evolution equation (3) was solved using the finite volume method.

2 Kinematics of Open Curves in hdCDD theory

The complexity of dislocation systems which can be described by the GND theory is very limited. The hdCDD theory allows the description of far more complex dislocation networks by adding an additional dimension (the dislocation direction) to each slip system, rendering it a four dimensional space [3]. The higher dimensional dislocation density vector reads $\mathbf{R} = (\rho, q)$, where $\rho$ is the scalar dislocation density, $I$ is the line direction and $q$ is the average curvature density. The main kinematic quantity of hdCDD is the second order dislocation density tensor

$$\alpha^{II} = \mathbf{R} \otimes b,$$ \hspace{1cm} (4)
which is defined in analogy to the GND case. The constraint for closed curves is \( \text{Div} \, \mathbf{R} = \text{div}(\rho \mathbf{l}) + \partial_t q = 0 \).

The evolution equations of the two density variables \( \rho \) and \( q \) are known for densities of closed curves [4]. The main result of this contribution are the evolution equations of open curve densities. They can likewise be derived using a Lie derivative and dropping the assumption \( \text{Div} \, \mathbf{R} = 0 \), yielding

\[
\begin{align*}
\partial_t \rho &= - \text{Div}(\rho \mathbf{V}) + \nu q - (v_b \cdot \mathbf{l}) \text{Div} \, \mathbf{R} \\
\partial_t q &= - \text{Div}(q \mathbf{V} - \nu \mathbf{R}) - \partial_b \text{Div} \, \mathbf{R},
\end{align*}
\]

where \( \mathbf{V} = (v, \nu) \) is the average higher dimensional dislocation velocity. In addition to the velocity \( v_b \), the rotational velocity \( \omega_b \) of the boundary points has to be specified. If the last term of each of the above equations is dropped, the original evolution equations for closed curves are recovered. This corresponds to a boundary point velocity which is orthogonal to the line direction and rotational boundary point velocity derived as the limiting value of the rotation of internal dislocation segments.

While the prescription of \( \omega_b \) is a challenging task, it allows a more general description of dislocation kinematics than the GND model. For example, the rotational boundary point velocity of the Frank-Read source shown in Figure 1 can be defined precisely. In the GND case, the rotational velocity of the boundary points would have to be prescribed by an artificial velocity profile along the dislocation line, as it is done in [2].

Possible boundary point velocities for the kinematic description of cross slip and Frank-Read source like multiplication are shown in Figure 2 and Figure 3, respectively. In the cross slip case, the boundary points are bound to move along the intersecting line of the involved slip systems. For a Frank-Read source, the rotational velocity would be assumed to be proportional to the dislocation velocity.

### 3 Discussion

The kinematics of open curves have been introduced for the GND theory and for the hdCDD theory. Future tasks are the kinematic description of phenomena such as cross slip, multiplication and annihilation, and the projection of the four dimensional evolution equations onto the three dimensional euclidean space in order to derive tractable theories without extra-dimensions [5].

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