Challenges in dislocation plasticity: Discrete vs. continuum, deterministic vs. stochastic models

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Fundamental problem in crystal plasticity: How to link dislocation physics and engineering elasto-plasticity?

- Not really relevant for traditional structural materials in macroscopic applications (phenomenology works just fine)
- Scale of interest: several μm sizes more and more important
- Influence of dislocations not negligible for small scale systems and microstructures: size effects, stochastic effects, hardening models

accuracy, physical foundation (atomistics and continuum elasticity)  computational efficiency, empirical foundation
Plastic deformation = motion (flux) of dislocations. Establish link between dislocation dynamics and continuum theory by casting dislocation dynamics into a continuum framework.

Potential advantages:

- Relating (size-dependent) plastic deformation to basic physical processes: interactions and transport of dislocations.
- Preserving the continuum setting (discrete dislocation dynamics scales badly and poses problems with general boundary conditions).
- Minimizing ad-hoc assumptions and free parameters (as used extensively in gradient- and other scale-dependent plasticity theories).
- Ideally: Deriving theory from discrete description through systematic coarse graining procedures fulfilling kinematic consistency requirements.
KRÖNER (1958): dislocation density tensor $\alpha$ with the properties

$$\alpha = \text{curl} \beta^{pl}$$

inhomogeneous plastic distortion causes a dislocation density

$$\text{div} \alpha = 0$$

dislocation lines do not start or end inside the crystal

$$\partial_t \alpha = \text{curl} \partial_t \beta^{pl}$$
evolution equation – not closed

• Limitations of the averaged density tensor $\alpha = \langle \alpha_d \rangle$

\[ l = \langle \delta_c \xi \rangle \]
\[ \alpha = \langle \alpha_d \rangle \]
\[ \partial_t \alpha \ldots \checkmark \]

$$b_{\text{net}} = -5\Delta x + 2\Delta x = -3\Delta x \checkmark$$

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Ekkehard Kröner 1999
(International Journal of Solids and Structures 38, 2001)

[...] We also wanted to show the obvious shortcomings of the present theory of elastoplasticity.

The greatest shortcoming is that the dislocation density tensor, no matter whether introduced through differential geometry or in the conventional way, measures the average dislocation density only and therefore, regards the internal mechanical state utmost incompletely.

In principle, this shortcoming could be overcome by reorientation of dislocation theory towards a statistical theory, but only with highest expenditure of computation.

Is it worthwhile to try that?
Requirements for a continuum theory of dislocation dynamics

a) Geometrical consistency: Theory must be consistent with classical continuum theory of dislocations (density measures must be able to characterize systems of curved and connected lines).

b) Kinematic consistency: Kinematic evolution and averaging should commute.

c) Correct representation of dislocation interactions (correct dynamics). Not trivial since a density-based theory cannot easily describe interactions on the segment level. Long-range interactions are automatically taken care of by (a)
The missing link in averaging dislocation kinematics

Most authors concentrated on averaging $\alpha$:

$$\alpha_d = \delta_c l \otimes b \quad \quad \alpha = \langle \alpha_d \rangle = \langle \delta_c l \otimes b \rangle$$

But the evolution of $\alpha$ needs the dislocation line density $\rho$:

$$\dot{\alpha}_d = -\text{curl}(\delta_c \mathbf{v}_d \times l \otimes b) \quad \quad \dot{\alpha} = \langle \dot{\alpha}_d \rangle = \text{curl}(\rho_{\mathbf{v}} n \otimes b)$$

$$\rho_d = \delta_c \quad \quad \rho = \langle \rho_d \rangle = \langle \delta_c \rangle$$

To close the description we need $\dot{\rho}_d$ and $\dot{\rho} = \langle \dot{\rho}_d \rangle = \text{??}$

A complete description of the dislocation kinematics needs to include an (average) description of the evolution of the dislocation line density
Averaging the evolution of the dislocation lines I: Single-orientation dislocation fields

It is not difficult to show that the discrete density has the evolution equation

$$\dot{\rho}_d = - \text{div}(\rho_d v_d) + \rho_d v_d k_d$$

An equivalent average equation holds for smoothly aligned dislocations (single-orientation dislocation fields):

$$\alpha = \rho \cdot \mathbf{l} \otimes \mathbf{b}$$
$$\alpha = - \text{curl}(\mathbf{v} \times \alpha)$$

$$\partial_t \mathbf{l} = (\partial_t v - v \text{div} \mathbf{l}) \frac{\mathbf{v}}{\|\mathbf{v}\|}$$
$$\dot{\rho} = - \text{div}(\rho \mathbf{v}) + \rho \nu k$$

Curvature information is needed for a closed description and can be retrieved from the direction field $\mathbf{l}$. However, what to do if dislocations in a given volume element can have arbitrary orientations? In this case,

$$\langle \rho_d v_d \rangle \neq \langle \rho_d \rangle \langle v_d \rangle$$
and similarly for $\langle \rho_d v_d k \rangle$
Averaging the evolution of dislocation lines II: Higher dimensional continuum theory of dislocations (HCDD)

Basic idea: Add additional dimensions (orientation coordinates) to the configuration space such that dislocations of different orientation located in the same volume element do not become entangled during averaging.

In the following: formulation for a single slip system, dislocation glide only, glide plane = xy plane.

Use as orientation coordinate the angle $\phi$ between line direction and Burgers vector $\mathbf{b} = (b,0)$

Generalized coordinate vector:
$$ \mathbf{r} = (p, \phi) $$

Generalized line direction:
$$ \mathbf{L}(p, \phi) = (l(\phi), k(p, \phi)) \quad \text{where} \quad l(\phi) = (\cos \phi, \sin \phi) $$
Generalised velocity

\[ \mathbf{V} = (\mathbf{v}, \vartheta) = (-v \sin(\varphi), v \cos(\varphi), \vartheta) \]

where \( \vartheta = \partial_t \varphi \) is the segment rotation velocity given by \( \vartheta = \nabla_L v \).

Define dislocation density tensor by analogy with classical tensor:

\[ \alpha_d = \delta_c \mathbf{1} \otimes \mathbf{b} \]
\[ \alpha^{II} = \delta_c \mathbf{L} \otimes \mathbf{b} \]

\[ \alpha = \langle \alpha_d \rangle = \langle \delta_c \mathbf{1} \otimes \mathbf{b} \rangle \]
\[ \alpha^{II} = \langle \alpha_d^{II} \rangle = \rho \mathbf{L} \otimes \mathbf{b} \]

The density function \( \rho = \rho(p, \varphi) \) is now a function of both spatial and orientation coordinates. As a consequence, the requirement of a common line direction of all segments in a spatial volume element can be dropped (segments in the same generalized volume element share by definition the same line direction).

As a new requirement, we have however to demand that all segments in the same generalized volume element share the same curvature.
Properties of the higher-dimensional dislocation density tensor

Higher-dimensional tensor contains curvature information:

\[ \alpha^{\Pi} = \rho \mathbf{L} \otimes \mathbf{b} \]

\[ \rho \mathbf{L} = (\rho_1, \rho_2) \]

The tensor can be written in terms of two scalar density fields:

- line density [length/volume] \( \rho \)
- curvature density [radians/volume] \( \rho_k =: q \)

The higher-dimensional divergence of the tensor vanishes:

\[ \hat{\nabla} \alpha^{\Pi} = \hat{\nabla} \rho \mathbf{L} \otimes \mathbf{b} = 0 \]

\[ \nabla_1 \rho + \partial_\phi q = 0 \]
Evolution equation for the higher-dimensional dislocation density tensor

Formulation in terms of differential forms results in evolution equations for the two scalar fields $\rho$, $q$:

\[
\begin{align*}
\alpha^\| (p) &= \rho(P) i_{L(p)} dV \otimes b \\
\frac{d}{dt} \alpha^\| &= 0 \\
\frac{\partial}{\partial t} \alpha^\| &= -\mathcal{L}_V \alpha^\|
\end{align*}
\]

For comparison: Classical theory for single-valued fields

\[
\begin{align*}
\partial_t \rho &= -\text{Div}(\rho \mathbf{V}) + \rho v_k \\
\partial_t q &= -\text{Div}(q \mathbf{V}) + \rho \nabla_L \nabla_L \mathbf{V}
\end{align*}
\]
Recovering the classical theory from the higher-dimensional formulation (single glide)

The classical tensor can be recovered by integrating over the line direction:

\[
\alpha = \int_0^{2\pi} \rho(\varphi)(\cos(\varphi), \sin(\varphi)) \sin(\varphi) \, d\varphi \otimes b =: \kappa \otimes b
\]

It can be shown that \( \text{div} \, \alpha = 0 \) follows from angular integration of \( \nabla_1 \rho + \partial_\varphi q = 0 \)

The plastic distortion rate is found as

\[
\dot{\beta}_{pl} = \int_0^{2\pi} \rho \nu \, d\varphi \otimes n \otimes b
\]

The theory is consistent: \( \dot{\alpha} = \text{curl} \, \dot{\beta}_{pl} \)
Interim Summary: A consistent theory of 3D dislocation kinematics

Comparison with DDD (nodal dislocation dynamics)

• Segment translation
• Segment rotation
• Introduction of new segments as curvature increases

All these kinematic aspects are covered in the proposed continuum theory.

Theory is geometrically consistent and comprises classical continuum theory.

But: theory is not yet dynamically closed. How is the dislocation velocity evaluated? In DDD: from local stress fields on segments, but in continuum theory?
From Kinematics to Dynamics: Constitutive relation for dislocation velocity

**Physical problem**: Deformation is driven by stresses on dislocation segments. Owing to short-range correlations in the dislocation arrangement, these stresses are (even on average) different from those at generic positions in space.

Mathematically speaking, the formulation of an averaged dynamic theory requires consideration of dislocation-dislocation correlations.

At this stage: Adopt a semi-phenomenological constitutive law:
Linear velocity law with line tension, friction stress, ‘back stress’.

\[
\begin{align*}
\nu &= \begin{cases} 
\frac{b}{B} \left( \tau - \tau_b - \tau_{lt} - \tau_y \right) & \text{if } \tau - \tau_b - \tau_{lt} > \tau_y \\
\frac{b}{B} \left( \tau - \tau_b - \tau_{lt} + \tau_y \right) & \text{if } \tau - \tau_b - \tau_{lt} < -\tau_y \\
0 & \text{otherwise}
\end{cases} \\
\tau_b &= -\frac{D G B}{\rho} \int \nabla \rho d \varphi, \quad \tau_{lt} = \frac{T q}{\rho}, \quad \tau_y = \alpha G b \sqrt{\rho},
\end{align*}
\]
Averaging the evolution of dislocation lines III: Simplified continuum theory CDD

Higher-dimensional theory is deficient from a practical point of view:

State space can be envisaged as direct produce of the real space and the unit circle (unit sphere if climb is allowed).

- 2 fields $\rho$, $q$ for each slip system
- In each point orientation space needs to be discretized
- Non-local (gradient) terms in the velocity

Consequence: We are dealing with a constitutive formulation of continuum plasticity with $O(10^2)$ internal variables in each spatial point.

Solution: Project theory back onto normal 3D space by appropriate expansions of the functions $\rho$, $q$, use higher-dimensional theory to derive equations of motion for the expansion coefficients which serve as new variables
Fourier representation of density fields

In case of glide only: Represent dependence of density fields on the directional angle in terms of a Fourier expansion:

\[
\rho(\varphi) = \frac{1}{2\pi} \left( \rho_t + \sum_{k=1}^{\infty} \rho_k^1 \cos(k\varphi) + \rho_k^2 \sin(k\varphi) \right)
\]

and similarly for \( q \).

- The zeroth order coefficient \( \rho_t \) is simply the total dislocation density (line length per unit volume)
- The first-order Fourier coefficients \( \rho_k^{1,2} \) are the densities of excess (geometrically necessary) edge and screw dislocation segments
Observations:

- Only the total curvature density $q_t$ needs to be considered independently. All higher-order Fourier coefficients can be derived from those of $\rho$ by angular integration of $\nabla_1 \rho + \partial_\phi q = 0$

- For direction-independent velocity, the strain rate is related to the total dislocation density
  \[ \dot{\beta}_{pl} = \rho_t v (n \otimes b) \]

- The classical dislocation density tensor is related to the dislocation density vector
  \[ a = \kappa \otimes b, \quad \kappa = [\kappa_1, \kappa_2] = [\rho_1^1, \rho_1^2] \]

Thus, the minimum number of coefficients needed for a closed theory are:

- Total dislocation density $\rho_t$
- Total curvature density $q_t$
- Components of the dislocation density vector (GND densities) $\kappa_1, \kappa_2$
Closure approximation:

Express higher-order coefficients in terms of lower-order terms. To this end we define

$$\kappa = \sqrt{k_1^2 + k_2^2}, \quad \varphi_\kappa = \arctan \frac{k_2}{k_1}$$

and set:

$$\begin{bmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{bmatrix} = \kappa \begin{bmatrix} \cos^2 \varphi_\kappa - 1/2 & \sin \varphi_\kappa \cos \varphi_\kappa \\ \sin \varphi_\kappa \cos \varphi_\kappa & \sin^2 \varphi_\kappa - 1/2 \end{bmatrix}$$

This is tantamount to assuming that all geometrically necessary dislocations have the same orientation.

Inserting into the higher-dimensional evolution equations produces and using this closure approximation a closed set of equations for 4 variables characterizing the dislocation system.
Evolution equations of CDD:

\[
\begin{align*}
\partial_t \rho_t &= -\nabla \cdot (v \kappa^\perp) + q_t v \\
\partial_t q_t &= -v \nabla \cdot \mathbf{q}^\perp - \frac{1}{2} \left[ (\rho_t + \kappa) \nabla^2_{\lambda \lambda} \mathbf{v} + (\rho_t - \kappa) \nabla^2_{\lambda \lambda} \mathbf{v} \right] \\
\partial_t \kappa &= \nabla \times (\rho_t v \mathbf{n})
\end{align*}
\]

\[
\begin{align*}
\kappa &= (\rho_1^1, -\rho_2^2, 0) = (\kappa \cos \varphi, \kappa \sin \varphi, 0) = \kappa_{\lambda \lambda} \mathbf{v} \\
\kappa^\perp &= (\rho_1^2, -\rho_1^1, 0) = (\kappa \sin \varphi, -\kappa \cos \varphi, 0) = \kappa_{\lambda \lambda}^\perp \mathbf{v} \\
q_t \rho_t &= \kappa q_t, \quad q_t^\perp \rho_t = \kappa^\perp q_t
\end{align*}
\]

- Kinematically consistent theory with 4 internal variables per slip system
- Complete description of inhomogeneous plastic distortion
- Acceleration by Factor $\sim 100$ against HCDD
- Still needed: constitutive equation for dislocation velocity
Constitutive law for dislocation velocity:

\[ \nu = \begin{cases} 
\frac{b}{B} \left( \tau - \tau_b - \tau_{lt} - \tau_y \right) & \text{if} \quad \tau - \tau_b - \tau_{lt} > \tau_y \\
\frac{b}{B} \left( \tau - \tau_b - \tau_{lt} + \tau_y \right) & \text{if} \quad \tau - \tau_b - \tau_{lt} < -\tau_y \\
0 & \text{otherwise}
\end{cases} \]

\[ \tau_b = -\frac{DGB}{\rho_i} \nabla_{1x} \kappa, \quad \tau_{lt} = \frac{Tq_t}{\rho_i}, \quad \tau_y = \alpha G b \sqrt{\rho_i} \]
Applications of (H)CDD

- Analytically solvable test cases: Spatially homogeneous behavior, spatially constant velocity field
- Spatially inhomogeneous deformation: Microbending, Microtorsion
- Confined plastic deformation: Square grain with impenetrable walls, system with impenetrable inclusion

Benchmarking of the performance of CDD solutions against analytical solutions, HCDD and DDD.
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Homogeneous loop distribution with Taylor-type hardening

\[
\begin{align*}
\partial_t \rho &= \rho v k, \\
\partial_t k &= -v k^2, \\
\partial_t \gamma &= \frac{2\pi}{0} \rho v b \, d\varphi \\
v &= B^{-1} b \left[ \tau(t) - (0.5\mu b) \sqrt{\rho(t)} - T/r(t) \right]
\end{align*}
\]

where \([\cdot]\) := \[\begin{cases} \cdot & \text{for } \cdot > 0 \\ 0 & \text{otherwise.} \end{cases}\]

- homogeneous distribution of circular loops, radius \(r\)
- homogeneous distribution of parallel glide planes
- distance of centers \(D \Rightarrow \rho = \frac{2\pi r}{D^2 A}\)
- quasi-static loading conditions
- different initial dislocation radii / const. initial density \(\rho_0 \equiv 5 \cdot 10^{11} \text{ m}^{-2}\)
- \(\mu = 10\text{GPa}, \ B = 50\text{Pa} \mu s, \ b = 0.22\text{nm}\)
Evolution of a distribution of loops under a spatially and temporally constant velocity field

Initial condition: \( r=1 \) loops distributed homogeneously over circular area of radius 2.5
Evolution of a distribution of loops

- Analytical: distribution with $r=2$
- CDD $r=1 \rightarrow 2$

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CDD \( r=2 \rightarrow 3 \), periodic bc

Analytical \( r=3 \)
• CDD $r=2 \Rightarrow 3.5$, open BC

Analytical $r=3.5$
CDD vs. HCDD: Dislocation density evolution in a quadratic grain with impenetrable boundaries
Comparison CDD-HCDD

Computation time on quad-core workstation (2.3MHz):
CDD 5 min
HCDD 9h
Torsion of a thin, single crystalline wire: CDD vs. DDD

initial microstructure
- surface sources at each surface emitting density with zero curvature

stress state and dislocation velocity
- surface sources at each surface emitting density with zero curvature
- backstress: statistical description of piling up of dislocations of the same sign:
- velocity (overdamped dislocation motion)

Identification of statistical parameter for back stress:

![Graph showing dislocation density vs. distance from neutral axis]
Bending of a free-standing thin film: CDD vs. DDD

- ‘Image stress’ boundary condition at surface chosen similarly to DDD
- Parameters ($\alpha, D$) fitted to DDD results
- Quasi-static loading

**Results:**
- Correct representation both of spatial strain distribution and of size effect
- Size-effect exponent ~ 1.2, in agreement with experimental data (Motz)
CDD: Shearing of a composite material

Composite material - a famous benchmark problem

[1] E. Van der Giessen and A. Needleman
Summary Part I

• By means of an 'excursion' into higher-dimensional spaces we could derive equations which describe the evolution of dislocation systems in terms of a small number of field variables.

• The kinematics of the dislocation evolution on a single slip system \((\mathbf{n}, \mathbf{b})\) can in many cases be described by three scalar variables:

  – Total dislocation density \(\rho_t\)
  – Curvature density \(q_t\)
  – Accumulated slip \(\gamma, \kappa\)

    (or its gradient, the GND density vector)

• While this does not work always (e.g. in case of strongly anisotropic dislocation mobility), we have now a systematic procedure for constructing more complex models.

• Theory performs well for many simple test cases.
Deformation of microscale specimens is characterized by size effects, but also by huge statistical variability of deformation rates and flow stresses.

Experimental stress-strain curves of Mo micropillars, d=0.5µm

Stress and dislocation density in DDD simulations of Al microbending
Size-dependent statistics of flow stresses (determined from 2D DDD simulations)

Yield stresses of finite systems are statistically distributed with a probability distribution that depends on system size as

\[ P_L(\sigma_y) = P[(\sigma_y - \sigma_y^\infty)L^{1/\nu}] \]

hence

\[ \langle \sigma_y \rangle = \sigma_y^\infty + CL^{-1/\nu} \]

Fitting method (Sethna):
Assume \( P \) (in log-normal form) and fit all distributions for different \( L \) simultaneously

\[ 1/\nu = 0.533 \]
Typical dynamics of plastic flow in DDD simulations:

- Intermittent deformation, discrete slip events (strain bursts, dislocation avalanches)
- Slip events are localized
- Statistical characterization: Statistics of stress and strain increments

Dislocation pattern in a simulated bending test (d=0.5µm, "pure bending")
Intermittent plastic flow:

- Load control: staircase-shaped stress-strain curves. Displacement control: serrated yielding

- Strain increments obey power law ('Gutenberg-Richter-law')

\[ p(\Delta \varepsilon) \propto \Delta \varepsilon^{-m} \]  

Mo Nanopillars, Zaiser, Schneider et al. 2008
Statistics of strain increments:

- Strain increments in 3D DDD simulations obey ‘universal’ statistics

\[ p(\Delta \varepsilon) = \Delta \varepsilon^{-m} \exp \left[ -\frac{\Delta \varepsilon}{\Delta \varepsilon_0} \right], \quad m = \frac{3}{2}, \quad \Delta \varepsilon_0 \propto \frac{E_b}{\Theta L} \]

- Universal: Does not depend on deformation mode, slip geometry, material parameters, simulation method, boundary conditions.

- Characteristic strain increment \( \varepsilon_0 \) ensures applicability of continuum models in macroscopic systems.
Statistics of stress increments (load control):

- Statistics is well described by Weibull distribution with exponent 0.8
- Mean stress increment between bursts decreases with increasing specimen size
- Little correlation between stress and strain increments
- Similar behavior in experiment (Mo), 2D und 3D-DDD simulation

Idea: develop stochastic models of plastic flow: replace computationally expensive dislocation dynamics simulations by equivalent stochastic processes
A Proposal towards modelling stochastic aspects of microplasticity: Stochastic continuum plasticity

Significant statistical scatter between experiments/simulations necessitates ensembles for evaluating the results of a given deformation process

Ensemble simulations by 3D-DDD are in general computationally not affordable for practical applications → develop stochastic continuum models

Basic idea (rate-independent case):

• Material = ‘composite’ consisting of volume elements with different deformation behavior
• Flow curve of one element = stochastic sequence of discrete events
• Generate flow curves using stochastic algorithm
• Couple elements through FEM
Example: Bending a long thin beam

aspect ratio 1:50, thickness 100\(\mu\)m.....0.1 \(\mu\)m, single crystalline [100]
boundary condition: increasing bending moment acts on beam ends
Individual realization and ensemble density:

d=100 µm  d=10 µm  d=1 µm  d=0.1 µm
Summary 2: Synthesis?

• Microplasticity requires dislocation based models

• Continuum models are desirable in view of
  ➢ Numerical efficiency and user-friendliness
  ➢ Dealing with general geometries and boundary conditions

• Dislocation-based continuum models have predictive power if compared to DDD ensembles (but not individual simulations!!!). The average quantities in these models must thus be considered as ensemble averages.

• The outcomes of individual simulations or experiments cannot be deterministically predicted. ‘Predicting the scatter’ needs new types of stochastic approaches that are yet in their infancy. How these approaches sit with CDD modelling is as yet rather unclear.

• Because of controlled initial conditions and complete microstructural information, DDD ensemble simulations can be an extremely powerful tool for:
  ➢ determining statistical properties of simulations and simulation ensembles
  ➢ parametrisation and validation of continuum models

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