A multi-scale approach to plasticity: the *Continuum Dislocation Dynamics* theory

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GAMM summer school *Multiscale Material Modeling*,
Bad Herrenalb, 2012

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Part 0: Introduction

Part I: Overview small-scale plasticity

Part II: The Continuum Dislocation Dynamics theory

1. Theoretical foundations
2. Numerical examples and validation
3. Outlook

Part III: Introducing... the DFG Forschergruppe *'Dislocation-based Plasticity'*

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Motivation: is **COPPER** = copper?

✓ centimeter-sized specimen can be used to predict meter-sized components

✗ Material behavior in small dimensions is not scale-invariant anymore

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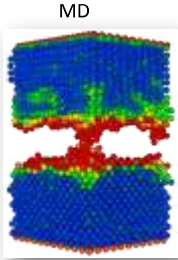
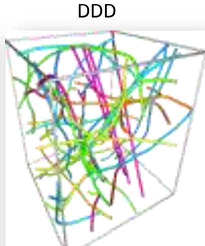
- How to predict plastic and hardening behaviour of components and devices?
- Scale of interest: several μm sizes becomes more and more important
- Influence of dislocations not negligible for:
  size effects, stochastic effects, physical hardening models

MD

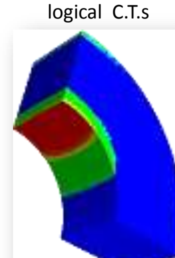


DDD



?

phenomeno-logical C.T.s



← higher accuracy, less assumptions | computational efficiency →

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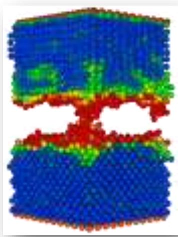

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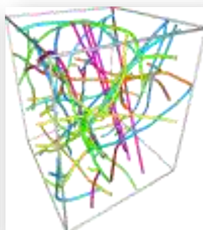
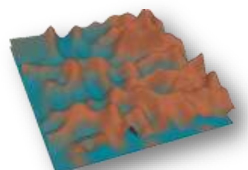


The Continuum Dislocation Dynamics Theory (CDD)



large range of μm, arbitrary dislocation density

phenomeno-logical C.T.s

← higher accuracy, less assumptions | computational efficiency →

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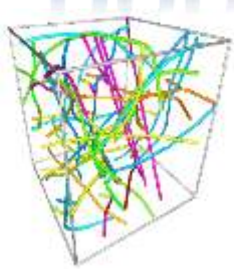
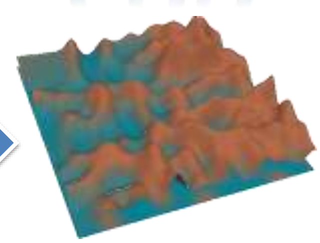
DDD



averaging →

CDD

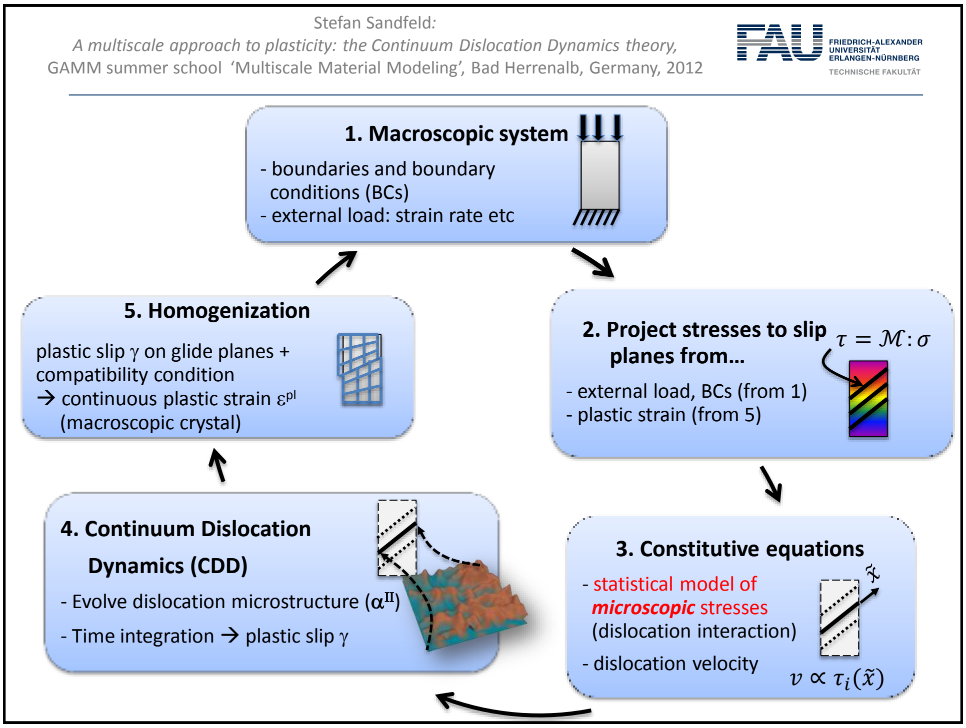


discrete dislocation dynamics

- movement of discrete lines
- internal stresses → analytical expressions
- limit: number of (interacting) lines

continuum dislocation dynamics

- evolution of dislocation density/curvature
- internal stresses →statistics
- computational cost independent of number of lines (density!)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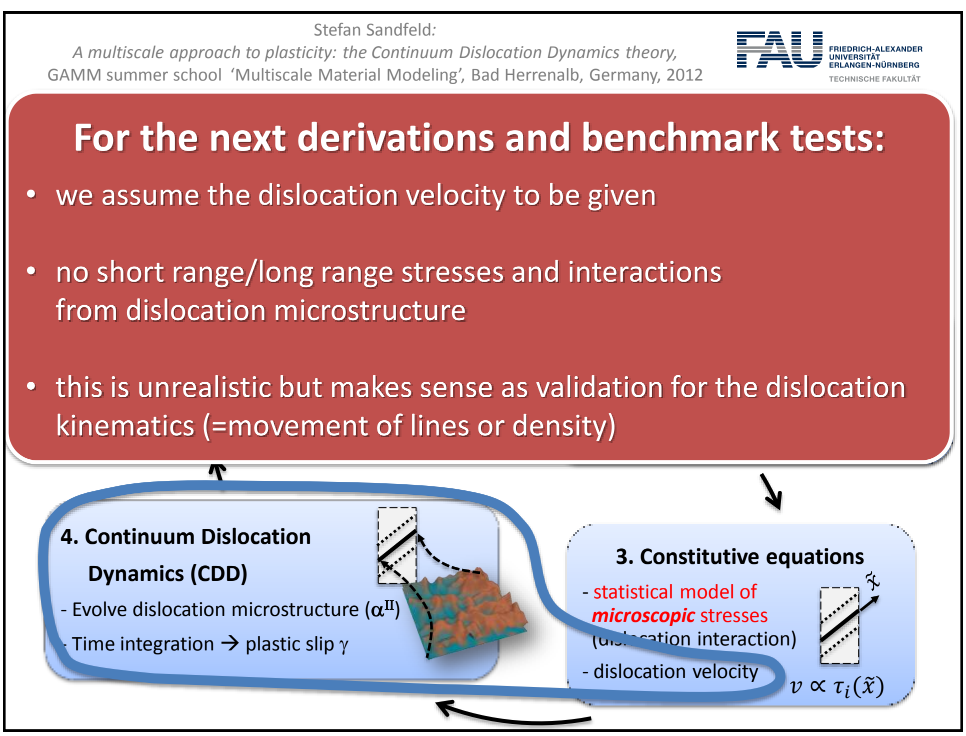
1. Macroscopic system
- boundaries and boundary conditions (BCs)
- external load: strain rate etc
2. Project stresses to slip planes from...
$\tau = \mathcal{M} : \sigma$
- external load, BCs (from 1)
- plastic strain (from 5)
3. Constitutive equations
- statistical model of *microscopic* stresses (dislocation interaction)
- dislocation velocity
$\tilde{x}$
$v \propto \tau_i(\tilde{x})$
4. Continuum Dislocation Dynamics (CDD)
- Evolve dislocation microstructure (α^{II})
- Time integration → plastic slip γ
5. Homogenization
plastic slip γ on glide planes + compatibility condition
→ continuous plastic strain ε^{pl} (macroscopic crystal)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For the next derivations and benchmark tests:
• we assume the dislocation velocity to be given
• no short range/long range stresses and interactions from dislocation microstructure
• this is unrealistic but makes sense as validation for the dislocation kinematics (=movement of lines or density)
4. Continuum Dislocation Dynamics (CDD)
- Evolve dislocation microstructure (α^{II})
- Time integration → plastic slip γ
3. Constitutive equations
- statistical model of *microscopic* stresses
interaction)
- dislocation velocity
$\tilde{x}$
$v \propto \tau_i(\tilde{x})$

The classical continuum theory of dislocations (Kröner, Nye, Bilby, Kondo in the ~1950s)

KRÖNER-NYE dislocation density tensor α:

$\alpha = \operatorname{curl}\beta^{\mathrm{pl}}$	inhomogeneous plastic distortion causes a dislocation density
$\operatorname{div}\alpha = 0$	dislocation lines do not start or end inside the crystal
$\partial_t\alpha = \operatorname{curl}\partial_t\beta^{\mathrm{pl}}$	evolution equation – generally not closed
$= \operatorname{curl}(-v\times\alpha)$	… - closed only for special case

Already Kröner was well aware of …
- the limitations of the dislocation density tensor
- the gap between dislocation physics and continuum plasticity in general

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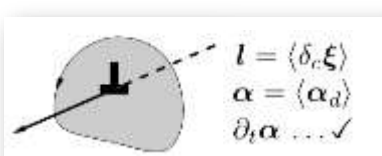
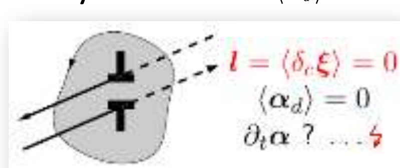
Limitations of the *averaged* density tensor $\boldsymbol{\alpha} = \langle\boldsymbol{\alpha}_d\rangle$





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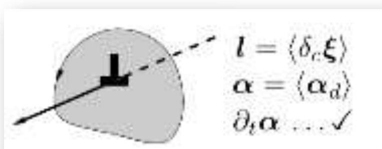

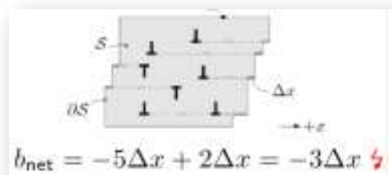

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In general, $\boldsymbol{\alpha}$ does not fulfill $\partial_t \boldsymbol{\beta}^{pl} = \mathbf{curl}(-\boldsymbol{v} \times \boldsymbol{\alpha})$ because…

$$\partial_t \alpha = -\operatorname{curl}\langle \partial_t \beta^{pl} \rangle = -\operatorname{curl}\left\langle \sum_{c} \delta_c v \times \xi_c \otimes \mathbf{b} \right\rangle \neq -\operatorname{curl} \sum_c \left(\langle \delta_c v \rangle \times \langle \xi_c \rangle \otimes \mathbf{b} \right)$$

velocity of line „c" — **Burgers vector** — **volume averaging < … >** — **line no. „c"** — **tangent of line „c"** — **average velocity** — **average line direction**

Applicability of the *averaged* Kröner-Nye tensor:

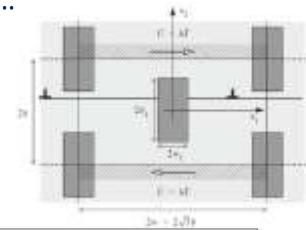
- OK: only 1 dislocation present (discrete case)
- OK: smooth line bundles with same tangent vector ξ and velocity $\boldsymbol{v}$
- BUT in general: averaging volume contains lines of different orientation
  → averaging yields $\rho_{GND} < \rho$

2D Continuum dislocation dynamics (Groma 1997):

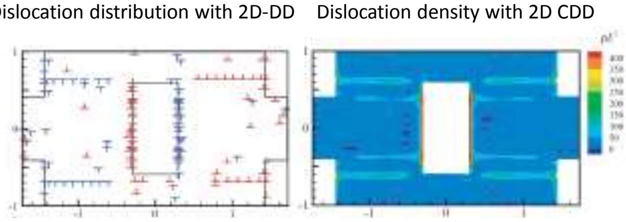
continuum theory of straight parallel edge dislocations, e.g. applied to…

Model composite

S. Yefimov et al. / J. Mech. Phys. Solids 52 (2004) 279-300



Dislocation distribution with 2D-DD   Dislocation density with 2D CDD



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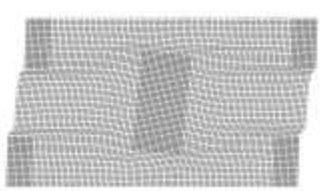
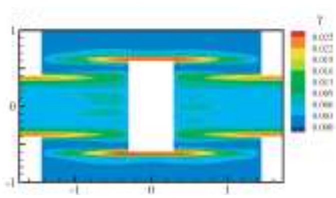
H. Cleveringa et al. / Acta Mater 1997; 45:3163.

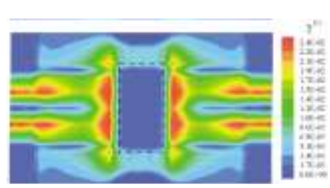


FE-mesh distortion with 2D-DD



Plastic strain with Groma CDD

S. Yefimov et al. / J. Mech. Phys. Solids 52 (2004) 279-300



Plastic strain with a model by M. Gurtin 2002

E. Bittencourt et al. / J. Mech. Phys. Solids 51 (2003) 281 – 310

Hochrainer's *Continuum Dislocation Dynamic* (CDD) theory

(HOCHRAINER, ZAISER & GUMBSCH, Phil. Mag. **87** (2007))

distinguish line segments according to their line orientation φ
→ lift of the line: $c(x,y) \rightarrow C(x,y,\varphi)$

⇩

average over the lift of the dislocation line
("controlled averaging")

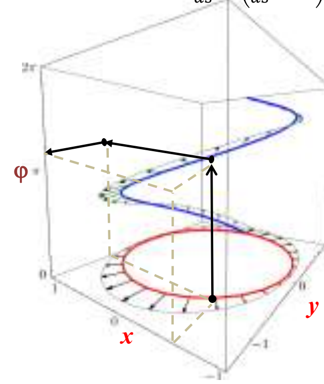
⇩

higher-dimensional continuum field description of dislocation microstructure

⇩

continuous representation of dislocation flow
→ dislocation density tensor of 2nd order α^{II}

tangent $L = \frac{dC}{ds} = \left(\frac{dc}{ds}, k(s)\right)$



Spatial dislocation loop (red) and lifted dislocation loop in the configuration space (blue)

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Hochrainer's *Continuum Dislocation Dynamic* (CDD) theory

Two main ingredients for the 'lift':

1. *generalised line direction* L
   $L_{(r,\varphi)} = (\cos\varphi, \sin\varphi, k_{(r,\varphi)})$
2. *generalised velocity* V
   $V_{(r,\varphi)} = (v\sin\varphi, -v\cos\varphi, \vartheta_{(r,\varphi)})$

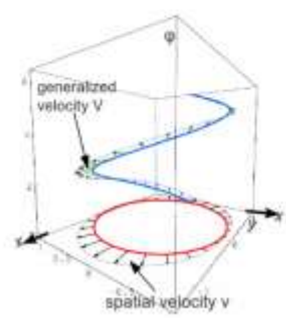

Figure: The arrows indicate the spatial velocity and generalized velocity along the respective spatial and lifted line.

with

k: lines' curvature
ϑ: rotational velocity
→ causing a line to move in orientation direction = rotation
→ basically a velocity gradient along the line

Can we obtain a closed form of the evolution equation for α^{II}?

$$\partial_t \alpha^{II} = -\mathrm{curl} \left\langle \sum_C \delta_C V \times \frac{\mathrm{d}C}{\mathrm{d}s} \otimes b \right\rangle = -\mathrm{curl} \sum_C \left(\langle \delta_C V \rangle \times \langle \tfrac{\mathrm{d}C}{\mathrm{d}s} \rangle \otimes b \right)$$

generalized velocity — gerneral. line direction

$$\partial_t \alpha^{II} = -curl \left(V \times \alpha^{II} \right)$$

...holds under much weaker assumptions: Dislocations in an averaging volume with same line direction...

1. **must have the same curvature**
2. **glide with the same magnitude of velocity**

KRÖNER: dislocation lines in an averaging volume must have same line direction φ the same velocity v

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CDD side-by-side with the classical Kröner theory

	CDD	Kröner
formal density definition	$\delta_c(r)=\int_c \delta(c(s)-r)\,\mathrm{d}s$	$\delta_C(r)=\int_C \delta(C(s)-(r,\varphi))\,\mathrm{d}s$
dislocation density tensor	$\alpha_{(r)}=\left\langle \sum_c \delta_c \frac{\mathrm{d}c}{\mathrm{d}s} \otimes b \right\rangle$	$\alpha^{II}_{(r,\varphi)}=\left\langle \sum_C \delta_C \frac{\mathrm{d}C}{\mathrm{d}s} \otimes b \right\rangle$
scalar dislocation density	$\rho=\left\Vert \left\langle \sum_c \delta_c \frac{\mathrm{d}c}{\mathrm{d}s} \right\rangle \right\Vert$	$\rho=\left\Vert \left\langle \sum_C \delta_C \frac{\mathrm{d}C}{\mathrm{d}s} \right\rangle \right\Vert_r$ (length of spatial pro-jection)
(average spatial/ generalized) line direction	$l=\left\langle \sum_c \delta_c \frac{\mathrm{d}c}{\mathrm{d}s} \right\rangle \cdot \rho^{-1}$	$L=\left\langle \sum_C \delta_C \frac{\mathrm{d}C}{\mathrm{d}s} \right\rangle \rho^{-1}=(l,k)$
density tensor	$\rightarrow \alpha_{(r)}=\rho\, l \otimes b$	$\rightarrow \alpha^{II}_{(r,\varphi)}=\rho\, L \otimes b$

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CDD side-by-side bith the classical Kröner theory

	CDD	Kröner
discrete disloc. current	$J^d_{(r)} = \sum_c \delta_c v^d \times \frac{dc}{ds} \otimes b$	$J^{d,II}_{(r)} = \sum_C \delta_C V^d \times \frac{dC}{ds} \otimes b$
dislocation density	$\alpha_{(r)} = \left\langle \sum_c \delta_c \frac{dc}{ds} \otimes b \right\rangle$	$\alpha^{II}_{(r,\varphi)} = \left\langle \sum_C \delta_C \frac{dC}{ds} \otimes b \right\rangle$
Evolution of disloc. density	$\partial_t \alpha_{(r)} = -\mathrm{curl} \langle J^d \rangle_{(r)}$	$\partial_t \alpha^{II}_{(r,\varphi)} = -\mathrm{curl} \langle J^{II,d} \rangle_{(r,\varphi)}$

→ both theories are very similar from a formal point of view

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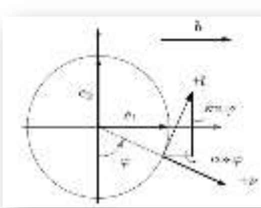
What do the governing equations look like?

→ if only dislocation glide in a slip plane is considered, α^{II} can be expressed in terms of scalar density ρ and average curvature k:

$$\alpha^{II}(r,\varphi) = \rho(r,\varphi) L(r,\varphi) \otimes b = \begin{pmatrix} \rho(r,\varphi) \cdot l^x(\varphi) \\ \rho(r,\varphi) \cdot l^y(\varphi) \\ \rho(r,\varphi) \cdot k(r,\varphi) \end{pmatrix} \otimes b \quad \text{with} \begin{cases} r \in \Re^2 \\ phi \in [0..2\pi) \end{cases}$$



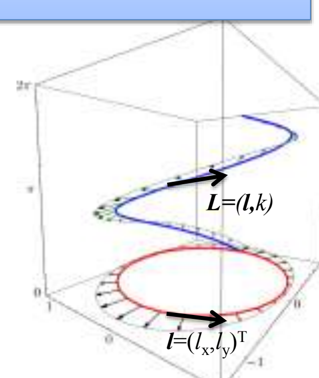
$l^x(\varphi) = \cos\varphi$, $l^y(\varphi) = \sin\varphi$ — components of tangent to the spatial loop

ρ: scalar density

k: average curvature

L: higher-dimensional line direction

b: Burgers vector



- evolution of dislocation density tensor 2^{nd} order α^{II} can be substituted by two scalar evolution equations:[1)]

1. *evolution of scalar density ρ*

$$\partial_t \rho = -\mathrm{div}\,(\rho \boldsymbol{v}) - \partial_\varphi(\rho\vartheta) + \rho v k$$

2. *evolution of mean dislocation curvature k*

$$\partial_t k = -v k^2 + \nabla_{\boldsymbol{L}}(\vartheta) - \nabla_{\boldsymbol{V}} k$$

RxRxS

- ρ and k both live in the configuration space $\mathbb{R} \times \mathbb{R} \times \mathbb{S}$
- v must be given, e.g. $v = \frac{b}{B}\left(\tau^{\mathrm{mf}} - \tau^{\mathrm{b}} \pm \tau^{\mathrm{f}}\right)$ if $|\tau^{\mathrm{mf}} - \tau^{\mathrm{b}}| \geq \tau^{\mathrm{f}}$
  → closure problem of dynamics

1) Sandfeld et al., Phil. Mag. (90) 2010

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Exploring the 2D system:
interpreting the components of the evolution equations

evolution of scalar density: $\partial_t \rho = -\underbrace{(\mathrm{div}(\rho \boldsymbol{v}) + \partial_\varphi(\rho\vartheta)}_{=\mathrm{Div}\,\rho V}) + \rho v k$

$\partial_t \rho = -\mathrm{div}(\rho \boldsymbol{v})\ldots$	spatial transport of density (spatial equation of continuity)
$\partial_t \rho = \ldots -\partial_\varphi(\rho\vartheta)\ldots$	transport of density in angular direction
$\partial_t \rho = \ldots -\rho v k$	increase of density due to line production of curved segments

transport in the configuration space

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Exploring the 2D system:
interpreting the components of the evolution equations

evolution of curvature: $\partial_t k = -vk^2 + \nabla_L(\vartheta) - \nabla_v(k)$

$\partial_t k = -vk^2 \ldots$	change of curvature as for an expanding/shrinking circular loop
$\partial_t k = \ldots + \nabla_L(\vartheta) \ldots$	change of rotational velocity along the lifted line (2nd derivative of velocity)
$\partial_t k = \ldots - \nabla_v(k)$	curvature change in direction of motion (Euler)

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Expanding loop with anisotropic velocity, $v=f(\varphi)$

$\partial_t \rho = -\mathrm{div}(\rho v) - \partial_\varphi(\rho \vartheta) + \rho v k, \quad \partial_t k = -vk^2 + \nabla_L(\vartheta) - \nabla_v(k)$

- ϑ: rotational velocity (vertical component of generalized velocity)

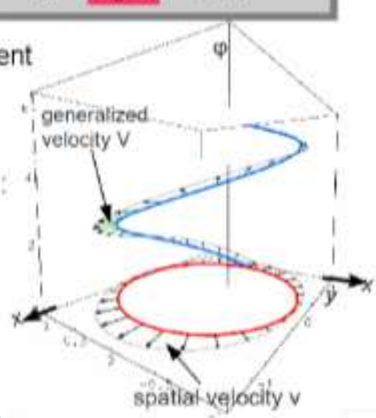
  $-\vartheta = \nabla_L v = \cos\varphi\, \partial_x v - \sin\varphi\, \partial_y v + k \partial_\varphi v$

- for $v = \mathrm{const}$ (expanding/shrinking loop):

  $\partial_\varphi(\rho \vartheta) = 0$

- anisotropic velocity $v = f(\varphi)$:

  $\partial_\varphi(\rho \vartheta) \neq 0$!



Anisotropic velocity → line rotation

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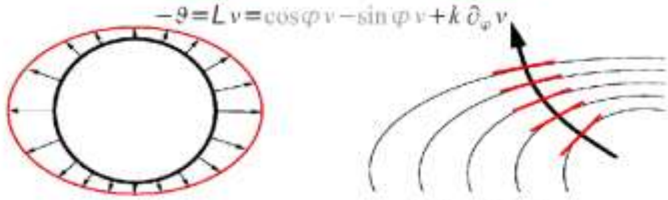
Exploring the Evolution Equations - Anisotropic velocity

Expanding loop: anisotropic velocity, v=f(φ)

$\partial_t \rho = -\mathrm{div}(\rho v) - \partial_\varphi(\rho \vartheta) + \rho v k, \quad \partial_t k = -v k^2 + \nabla_L(\vartheta) - \nabla_L(k)$

$-\vartheta = L v = \cos\varphi\, v - \sin\varphi\, v + k\, \partial_\varphi v$



(spatial) velocity along the line

rotation of a line segment (red) during loop expansion due to anisotropic velocity law

A multiscale approach t
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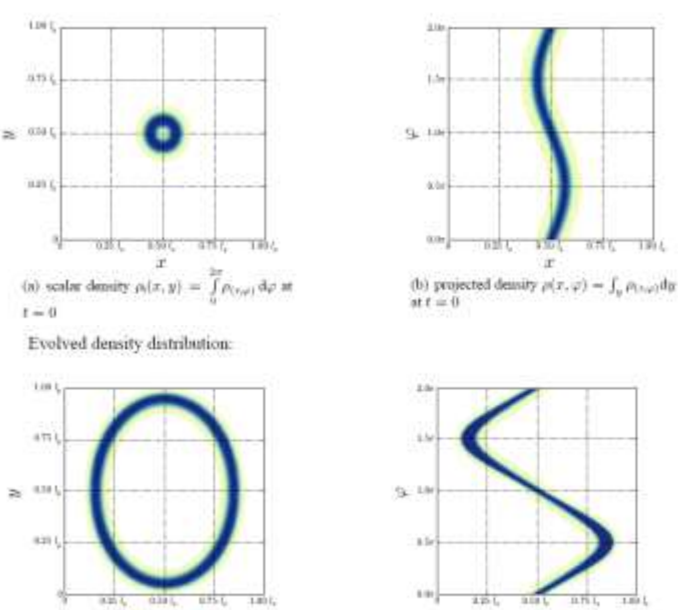
Expansion of a dislocation loop in a anisotropic stress field



(a) scalar density $\rho(x, y) = \int_0^{2\pi} \rho_{(x,y,\varphi)}\,d\varphi$ at $t = 0$

(b) projected density $\rho(x, \varphi) = \int_y \rho_{(x,y,\varphi)}\,dy$ at $t = 0$

(c) scalar density $\rho(x, y)$ at $t = 180$

(d) projected density $\rho(x, \varphi)$ at $t = 180$

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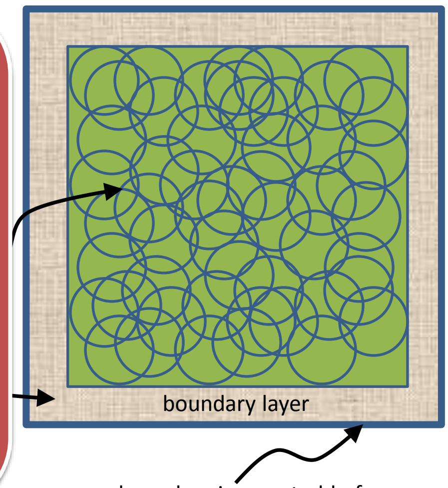
Boundary conditions in CDD – analyzing the path of dislocations

in fact, we only have density representing a loop distribution, there are NO discrete dislocation loops!



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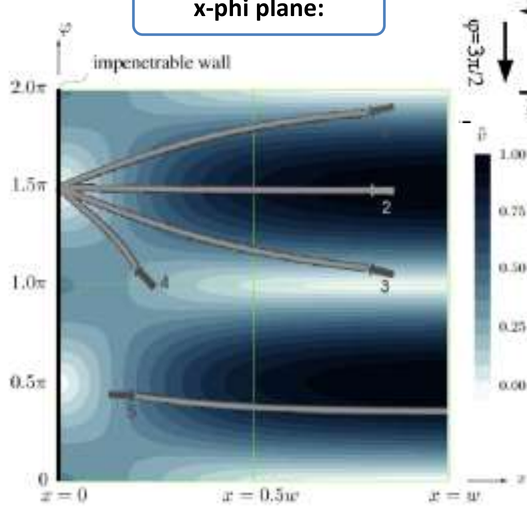
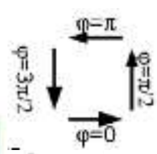
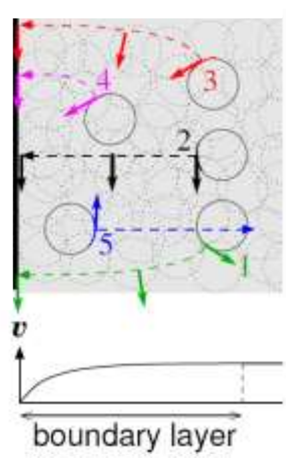
Boundary conditions in CDD – analyzing the path of dislocations

x-phi plane:

x-y plane:







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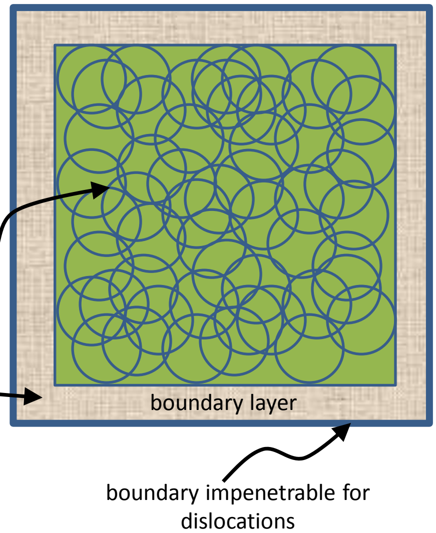
Quadratic ‚grain' with impenetrable boundaries

Initial values:
- circular dislocation loops , radius r = 2µm
- all loops stem from e.g. Frank-Reed sources (→ plastic slip)
- total density ρ= 0.1 · $10^{13}m^{-2}$

Velocity and boundaries:
- v=const in the inner part
- v → 0 in the boundary region



boundary conditions are realized as flux boundary conditions

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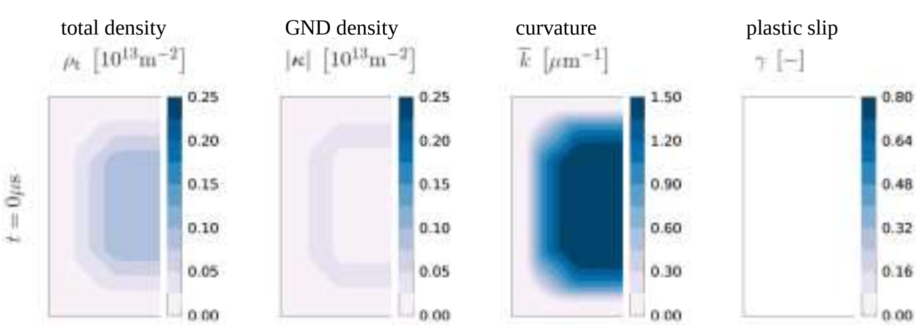
Quadratic ‚grain' with impenetrable boundaries

Dislocation field quantities for the left half of a quadratic cell (l=20µm) with impenetrable boundaries:



Initial values:
- circular dislocation loops , radius r = 2µm
- total density ρ= 0.1 · $10^{13}m^{-2}$

Velocity and boundaries:
- constant velocity in the inner part
- velocity → 0 in the boundary region

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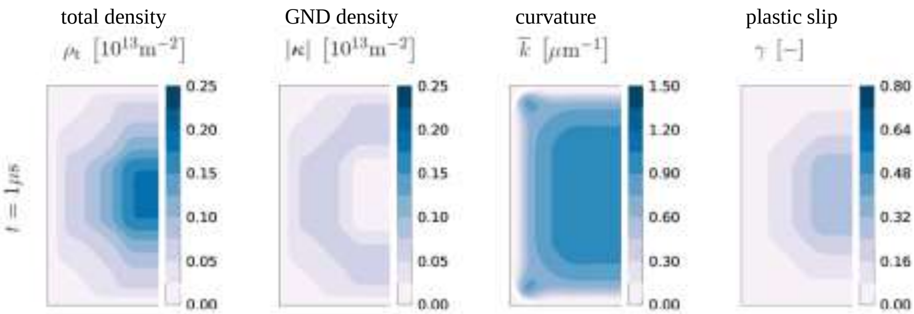

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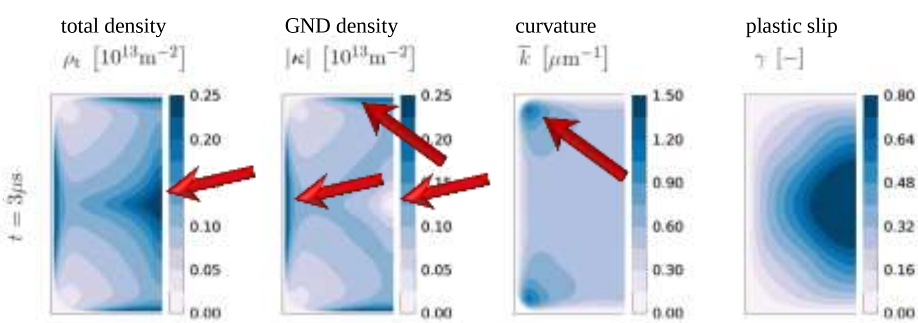

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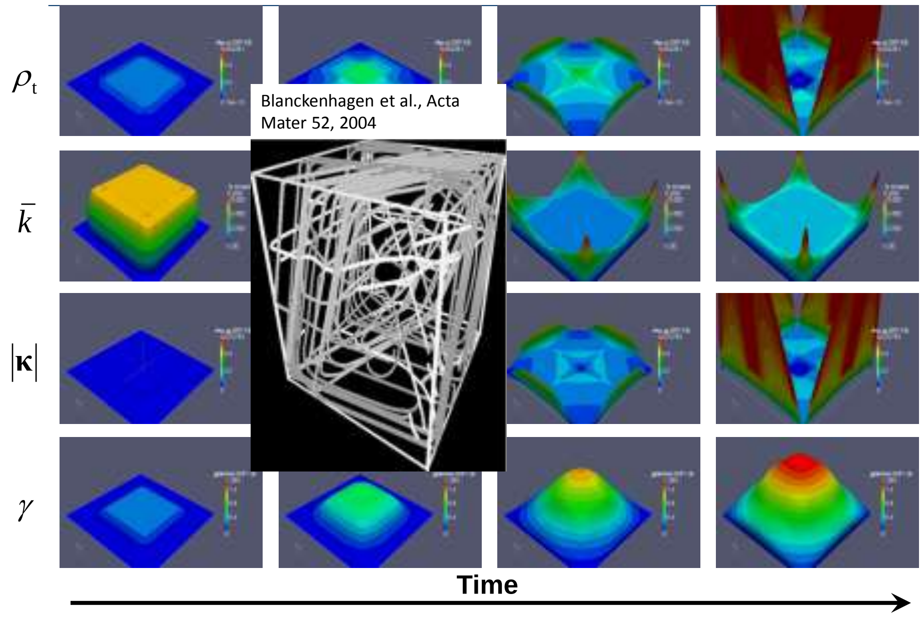

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Simplifying the higher-dimensional CDD

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Reduction of degrees of freedom by integration over orientation space (HOCHRAINER et al. 2009, AIP Conf. Proc. 1168(1))

$$\alpha^{\mathbf{II}}(r,\varphi) = \rho(r,\varphi) L(r,\varphi) \otimes b = \begin{pmatrix} \rho(r,\varphi)\cdot l^x(\varphi) \\ \rho(r,\varphi)\cdot l^y(\varphi) \\ \rho(r,\varphi)\cdot k(r,\varphi) \end{pmatrix} \otimes b \quad \text{with} \begin{cases} r \in \Re^2 \\ phi \in [0..2\pi) \end{cases}$$

$$l^x(\varphi) = \cos\varphi$$

$$l^y(\varphi) = \sin\varphi$$

Integration over orientation space

$$\rho^{\mathbf{t}}(r) = \int_0^{2\pi} \rho(r,\varphi)\,\mathbf{d}\varphi, \qquad q^{\mathbf{t}}(r) = \int_0^{2\pi} \rho(r,\varphi)\cdot k(r,\varphi)\,\mathbf{d}\varphi$$

$$\kappa^{1}(r) = \int_0^{2\pi} l^x(\varphi)\rho(r,\varphi)\,\mathbf{d}\varphi, \qquad \kappa^{2}(r) = \int_0^{2\pi} l^y(\varphi)\,\rho(r,\varphi)\,\mathbf{d}\varphi$$

$$\in \Re^2$$

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$$l^x(\varphi) = \cos\varphi$$

$$L = \int_V \rho\, dV$$

Integration over orientation space

$$N = \frac{1}{2\pi}\int_{\Omega\times S^1} q\, d\mathcal{V}$$

$$\rho^{\mathbf{t}}(r) = \int_0^{2\pi} \rho(r,\varphi)\,\mathbf{d}\varphi, \qquad q^{\mathbf{t}}(r) = \int_0^{2\pi} \rho(r,\varphi)\cdot k(r,\varphi)\,\mathbf{d}\varphi$$

$$\kappa^{1}(r) = \int_0^{2\pi} l^x(\varphi)\rho(r,\varphi)\,\mathbf{d}\varphi, \qquad \kappa^{2}(r) = \int_0^{2\pi} l^y(\varphi)\,\rho(r,\varphi)\,\mathbf{d}\varphi$$

$$\in \Re^2$$

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$$l^x(\varphi) = \cos\varphi$$

$$l^y(\varphi) = \sin\varphi$$

Integration over orientation

11 and 12-components of Kröner tensor α

$$\kappa^1(r) = \int_0^{2\pi} l^x(\varphi)\rho(r,\varphi)\,\mathbf{d}\varphi, \qquad \kappa^2(r) = \int_0^{2\pi} l^y(\varphi)\rho(r,\varphi)\,\mathbf{d}\varphi \quad \in \Re^2$$

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Derivation of simplified evolution equations:

$$\partial_t \boldsymbol{\alpha}^{\mathrm{II}}{}_{(\boldsymbol{r},\varphi)} = -\mathrm{curl}\left(\boldsymbol{V}_{(\boldsymbol{r},\varphi)} \times \boldsymbol{\alpha}^{\mathrm{II}}{}_{(\boldsymbol{r},\varphi)}\right) \qquad \text{hdCDD}$$

Assumption:
v and *k* are orientation independent

sCDD

$$\partial_t \rho^{\mathrm{t}} = -\left(\partial_x(v\kappa^2) - \partial_y(v\kappa^1)\right) + v\rho^{\mathrm{t}}\bar{k}$$
$$= -\mathrm{div}(v\boldsymbol{\kappa}^{\perp}) + v\rho^{\mathrm{t}}\bar{k}$$
$$\partial_t \boldsymbol{\kappa} = \left(-\partial_y(v\rho^{\mathrm{t}}),\ -\partial_x(v\rho^{\mathrm{t}})\right)$$
$$\partial_t \bar{k} = -v\bar{k}^2 - \frac{1}{2}\left(\frac{\rho^{\mathrm{t}}+\rho^{\mathrm{G}}}{\rho^{\mathrm{t}}}\nabla_{l,l}v + \frac{\rho^{\mathrm{t}}-\rho^{\mathrm{G}}}{\rho^{\mathrm{t}}}\nabla_{v,v}v\right) - \frac{1}{\rho^{\mathrm{t}}}\left(\bar{k}\boldsymbol{\nabla}_{\boldsymbol{\kappa}_v} v - v\boldsymbol{\nabla}_{\boldsymbol{\kappa}_v}\bar{k}\right)$$

dislocation velocity $v = \frac{b}{B}\tau_{\text{res.}}$ with b: Burgers vector, B: drag coefficient

$$\tau_{\text{resulting}} = \begin{cases} \operatorname{sgn}(\tau_0)\left(|\tau_0| - |\tau_y|\right) & \text{if } |\tau_0| > |\tau_y| \\ 0 & \text{otherwise} \end{cases} \quad \text{where} \quad \tau_0 = \tau_{ext} + \tau_{sc} - \tau_b - \tau_{lt}$$

τ_{ext} **resolved shear stress** (from elastic BVP, e.g. strain rate)

τ_{sc} **self-consistent stress** (from elastic eigenstrain problem)

$\tau_b \approx \nabla \rho^G \approx \nabla^2 \gamma$ **back stress** (short range interaction) (proportional to gradient of GND density)

$\tau_{\text{lt}} = Gb^2k$ **line tension** (short range interaction) (proportional to average curvature)

$\tau_y \approx \rho^{1/2}$ **yield stress** (proportional to square root of total density)

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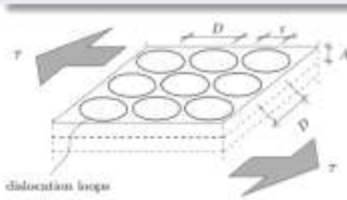
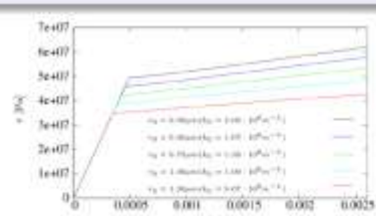
Homogeneous loop distribution with Taylor-type hardening

$$\partial_t \rho = \rho v k, \quad \partial_t k = -v k^2, \quad \partial_t \gamma = \int_0^{2\pi} \rho v b \, d\varphi$$

$$v = B^{-1} b \left\lfloor \tau(t) - (0.5\mu b)\sqrt{\rho(t)} - T/r(t) \right\rfloor \quad \text{where } \lfloor \cdot \rfloor := \begin{cases} \cdot & \text{for } \cdot > 0 \\ 0 & \text{otherwise.} \end{cases}$$





- 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 $\rho_0 \equiv 5 \cdot 10^{11}\ \text{m}^{-2}$
- $\mu = 10\text{GPa}$, $B = 50\text{Pa}\mu\text{s}$, $b = 0.22\text{nm}$

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Bending of a thin, single crystalline film

Geometry and details of the double-slip bending system

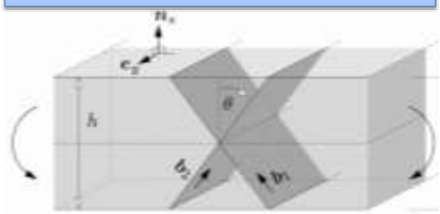

Figure 1: Geometry

- „flux" boundary conditions similar to DDD
- 2 slip systems
- 2 microscopic stress components: Taylor-type yield stress and back stress
- quasi-static load steps

Size dependence of the flow stress for different surface strains

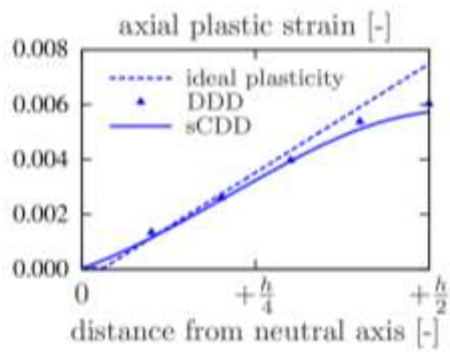

Figure 2: size effect and strain profiles

S. Sandfeld et al., *Philos. Mag.* **90**, 3697 (2010), S. Sandfeld et al., *J. Mater. Res.* **26**, 623 (2011).

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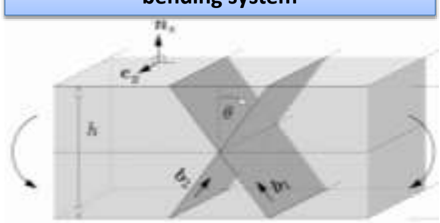


Figure 1: Geometry

- only 2 free parameter for Taylor-type yield stress and back stress (quality: almost universal constants)
- strain profiles and size-effect reproduced (match with experiments and DDD)

Size dependence of the flow stress for different surface strains

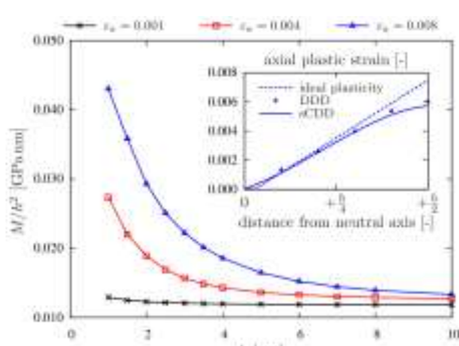


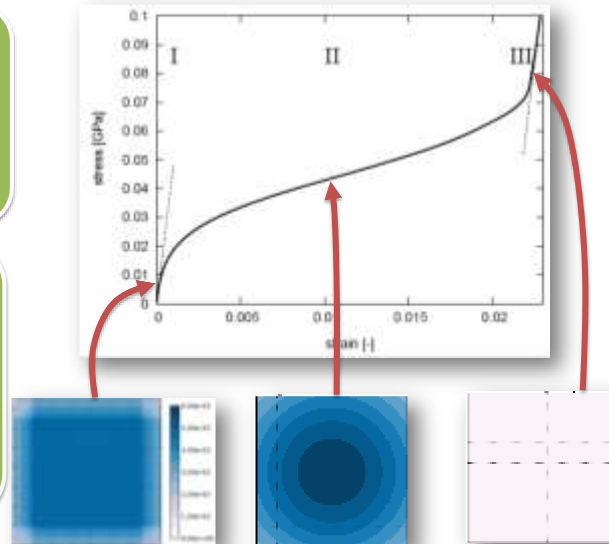
Figure 2: size effect and strain profiles

S. Sandfeld et al., *Philos. Mag.* **90**, 3697 (2010), S. Sandfeld et al., *J. Mater. Res.* **26**, 623 (2011).

Mechanical annealing (‚dislocation starvation')

- compression test of a nano pillar
- 2 symm. slip systems
- initially homogenous loop distribution
- open boundaries
- Taylor-type flow stress

- initially: elastic response (regime I)
- plastic activity = loop expansion/outflux (regime II)
- all dislocations left = elastic response (regime III)



total dislocation density

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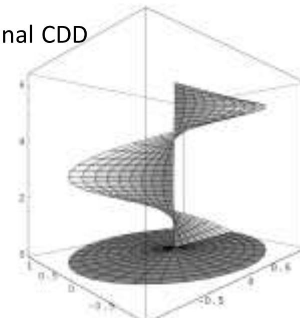
Intermittent plastic behavior:

Dislocation nucleation within the CDD theory

- **Point of departure for derivation**: higher-dimensional CDD
- **Extra source-terms**:

$\partial_t \rho_{src} = \dot{q} k_{src}$ and $\partial_t k_{src} = \frac{\dot{q}}{\rho} k_{src}(k_{src} - k)$

$\dot{q}$: rate of plastic deformation due to sources
k_{src}: initial curvature of newly formed loops



Newly introduced loop in physical space (bottom) and in the configuration space (T. Hochrainer, PhD thesis, 2006)

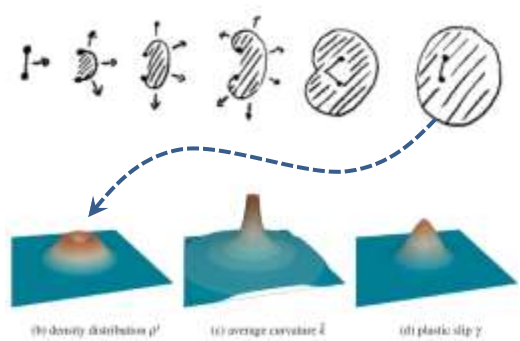
Averaging the above CDD evolution equations yields the **simplified CDD equations with sources**:

$$\partial_t \rho^{t} = -\mathrm{div}(v\boldsymbol{\kappa}^{\perp}) + v\rho^{t}\bar{k} + \dot{\rho}_{src}$$
$$\partial_t \boldsymbol{\kappa} = \left(-\partial_y\left(v\rho^{t} + \dot{\rho}_{src}/\bar{k}_{src}\right),\ -\partial_x\left(v\rho^{t} + \dot{\rho}_{src}/\bar{k}_{src}\right)\right)$$
$$\partial_t \bar{k} = -v\bar{k}^2 - \frac{1}{2}\left(\frac{\rho^{t}+\rho^{G}}{\rho^{t}}\boldsymbol{\nabla}_{l,l}v + \frac{\rho^{t}-\rho^{G}}{\rho^{t}}\boldsymbol{\nabla}_{v,v}v\right) - \frac{1}{\rho^{t}}\left(\bar{k}\nabla_{\boldsymbol{\kappa}_v}v - v\nabla_{\boldsymbol{\kappa}_v}\bar{k}\right)$$
$$\ldots + \dot{\rho}_{src}\left(k_{src} - \bar{k}\right) - \Delta\dot{\rho}_{src}/(2k_{src})$$

Two possible types of nucleation processes in CDD

1. **Quasi-discrete sources**
   (S. Sandfeld et al., AIP Conf. Proc., Vol. 1389, 1531-1534, 2011)

   - similar to the discrete Frank-Read sources
   - …but: initial bowing-out is not considered
   - continuum source emitts density with curvature and plastic slip ($\Delta\rho_{\text{src}}$ instead of $\dot{\rho}_{\text{src}}$!!)



   - activation of the source: *average* shear stress under source area **>** critical shear stress

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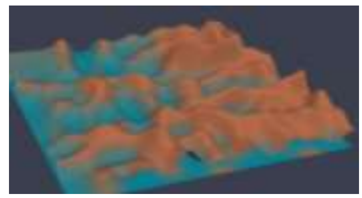
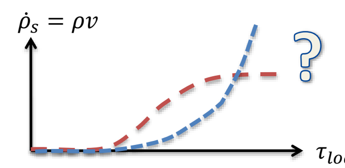
Two possible types of nucleation processes in CDD:

2. Continuous "source field"

- average description of many Frank-Read sources
- each point of the continuum: influx of density (→ $\dot{\rho}_S$) with certain curvature (and plastic slip)



Temporal averaging results in:
- no discrete activation
- (after some threshhold…) influx proportional to local stress



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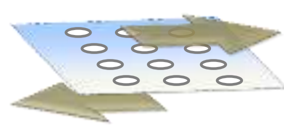
- **System:**
  - 0-dimensional = homogeneous in x and y direction
  - constant strain rate $\dot{\varepsilon} = 10^5 s^{-1} \Rightarrow \dot{\tau}_{\rm ext} = G\dot{\varepsilon}$
  - material parameter : b=0.256nm, B=5.e-6GPa/µs, E=128GPa, ν=0.33, T=4GPa/nm², a=0.4

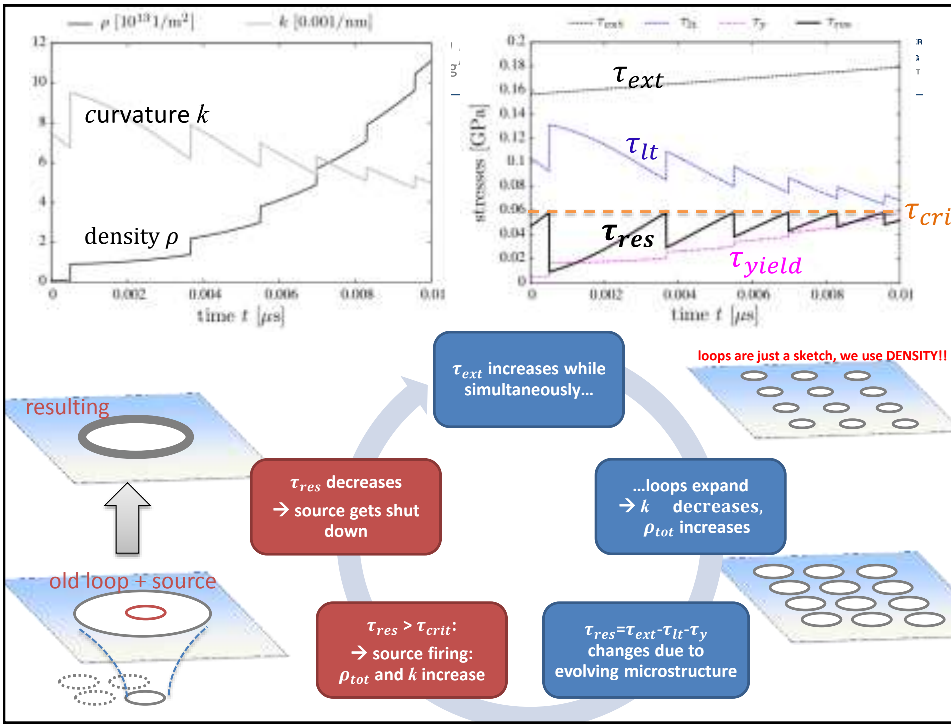


- **Velocity** is a function of τ_{ext}, $\tau_{lt} = Tk$ and $\tau_y = aGb\sqrt{\rho}$

- **Evolution equations** ($\dot{\rho}_S$ such that 1 loop is emitted upon activation)
  … source inactive: $\dot{\rho}_{\rm t} = v\rho_{\rm t}\bar{k}$ $\quad \dot{\bar{k}} = -v\bar{k}^2$ $\quad \dot{\gamma} = v\rho_{\rm t}|b|$
  … source active: $\dot{\rho}_{\rm t} = v\rho_{\rm t}\bar{k} + \dot{\rho}_{\rm s}$ $\quad \dot{\bar{k}} = -v\bar{k}^2 + \frac{\dot{\rho}_{\rm s}}{\rho_{\rm t}}(k_{\rm s} - k)$ $\quad \dot{\gamma} = (v\rho_{\rm t} + \dot{\rho}_{\rm s}/k_{\rm s})|b|$

- **Initial conditions**: $\rho_{\rm t,0} = 10^{12}/{\rm m}^2$ $\quad k_0 = 0.005/{\rm nm}$ $(r_0 = 200$ nm)
  $\rho_{\rm s} = 10^{12}/{\rm m}^2$ $\quad k_{\rm s} = 0.00455/{\rm nm}$ $(r_0 = 220$ nm)

- **Source parameters**: $\tau_{\rm crit} = \dfrac{T}{b \cdot l_{src}} = 58.85\,{\rm MPa}$



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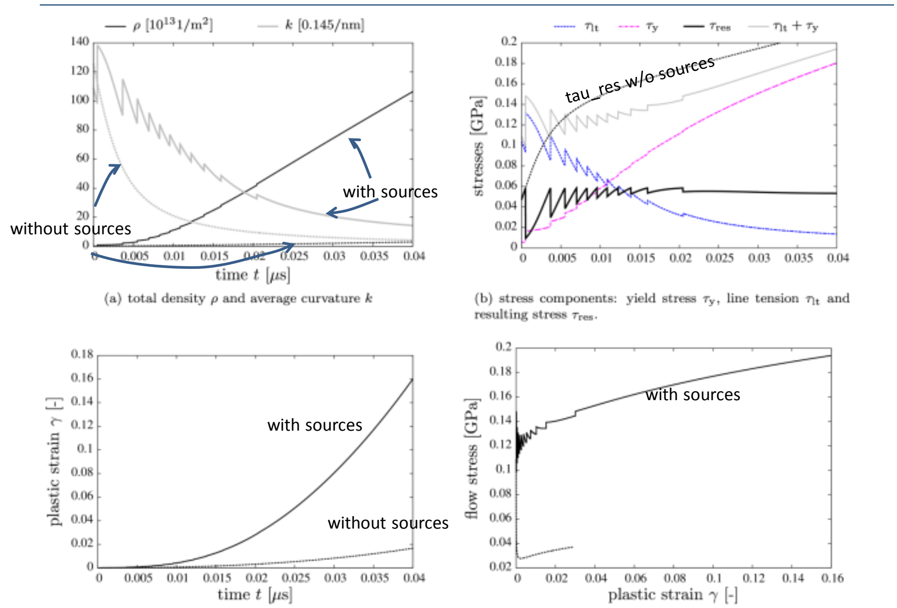

(a) total density ρ and average curvature k

(b) stress components: yield stress τ_y, line tension τ_{lt} and resulting stress τ_{res}.

(c) evolution of accumulated plastic strain γ

(d) stress $\tau_{lt} + \tau_y$ vs plastic strain

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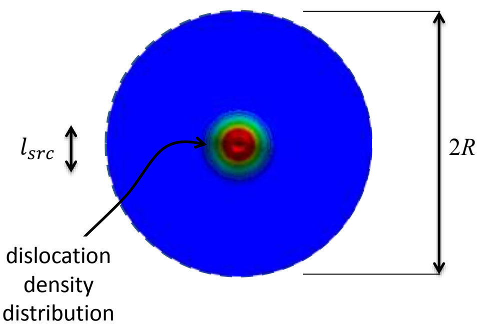
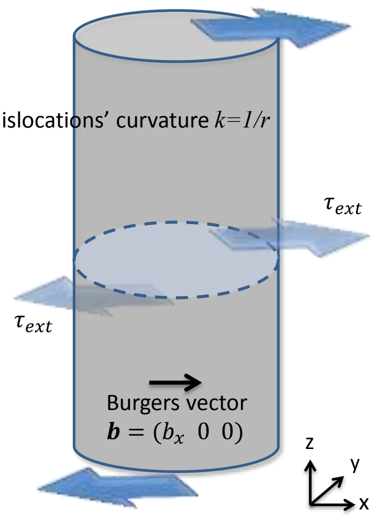
Quasi-discrete sources: the system

- circular slip plane (radius R) with constant resolved shear stress τ_{ext}
- pure edge source, source length l_{src}
- critical stress for activation $\tau_{crit} = {}^{2Gb}/_{l_{src}}$
- line tension (simplified): $\tau_{lt} = Gb^2 k$ with the dislocations' curvature $k=1/r$
- pure edge source: loop diameter ~ $1.5 * l_{src}$





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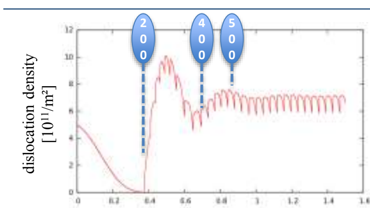
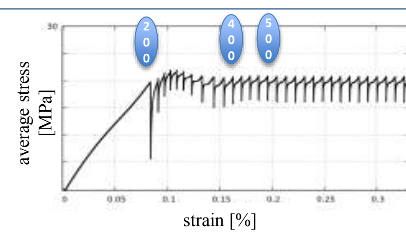
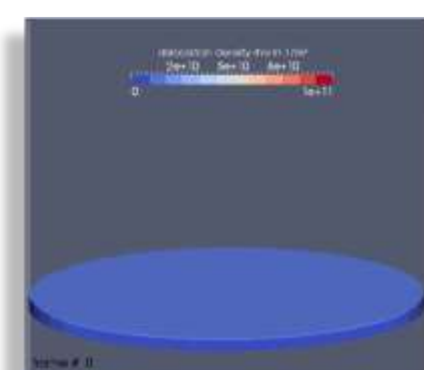
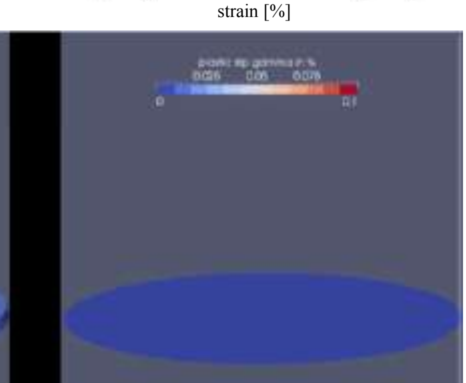
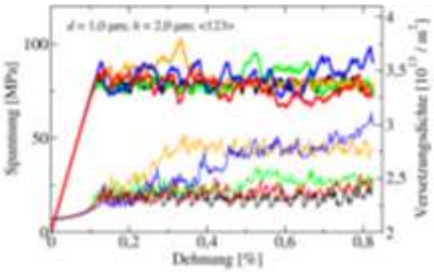


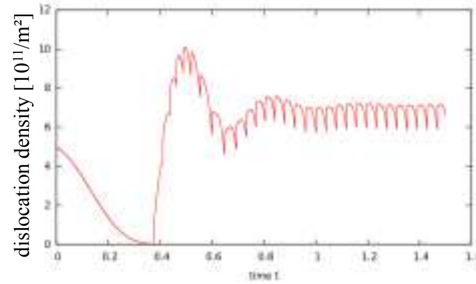


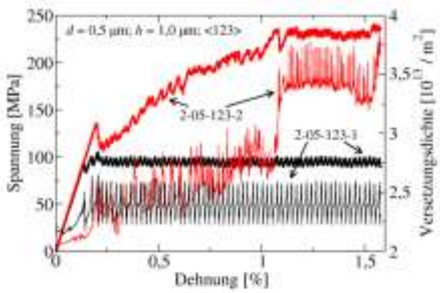


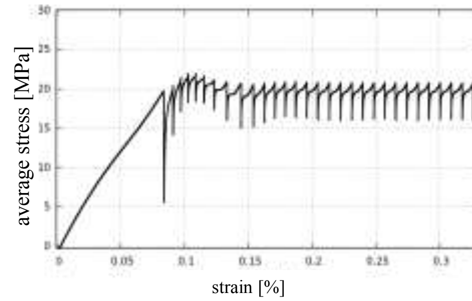


Here, the back stress plays an important role for activating the source









J. Senger 2009, PhD thesis …some qualitative comparisons

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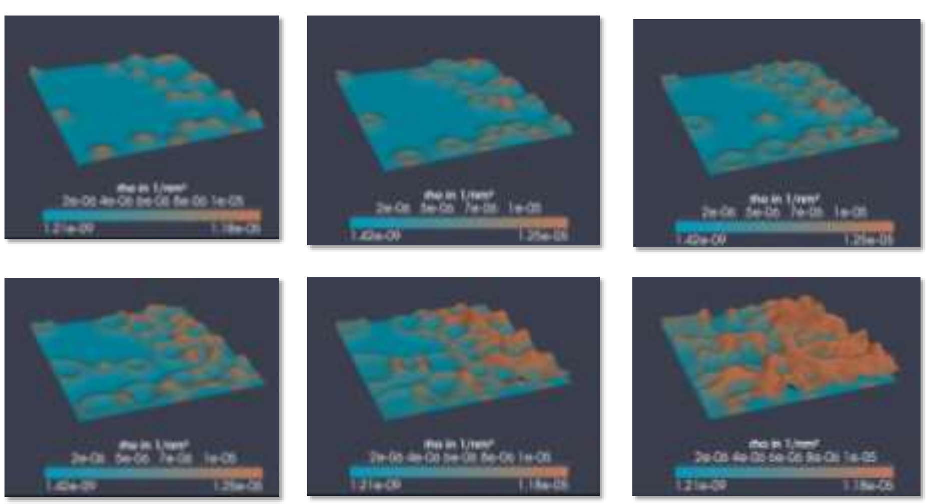
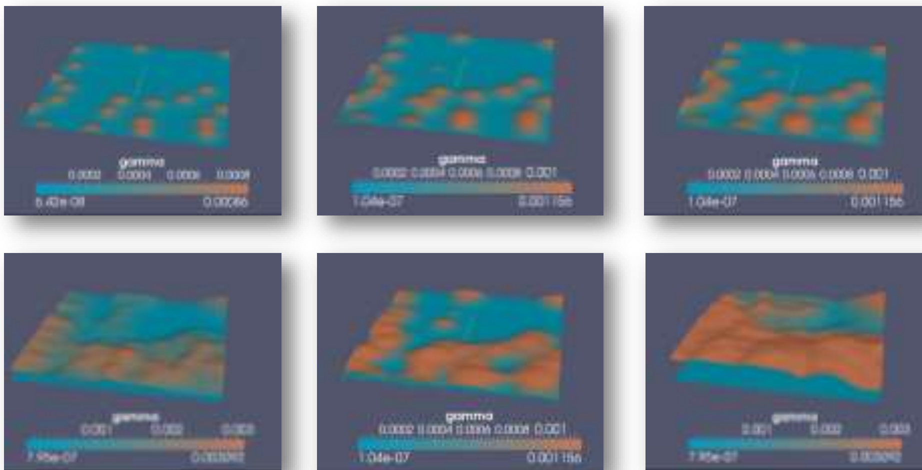
snapshots of density evolution in a 2D source distribution



snapshots of accumulated plastic slip in a 2D source distribution



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Summary and Outlook

- CDD contains the kinematics of curved lines - line curvature is THE key ingredient!
- Intermittend plastic activity as well as continuous fluxes can be represented in a straightforward manner
- boundary conditions can be easily included
- hdCDD even allows for anisotropic velocity law (e.g. edge/screw anisotropy or mixed FR source)

- More work to be done on systematically simplifying evo. eqns + benchmarking
- Full FE coupling with full FCC slip systems
- Analyzing DDD configurations to extract internal stresses, short/long-range stress