The Evolution of Dislocation Density in a Higher-order Continuum Theory of Dislocation Plasticity

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The growing demand for physically motivated continuum theories of plasticity has led to an increased effort on dislocation based field descriptions. Only recently rigorous techniques have been developed by T. Hochrainer for performing meaningful averages over systems of moving, curved dislocations, which can be described by a higher order dislocation density tensor. Within this thesis we rewrite this continuum theory of dislocations using exclusively standard vector and tensor calculus. This formulation is much more accessible (although still defined in a higher order configuration space) than the original formulation which uses differential forms and higher order currents. This formulation then serves as the starting point for the numerical exploration of the continuum theory where we cover simple benchmark problems, which allow for verification with analytical solutions. This already demonstrates that within this theory it is possible to predict dislocation kinematics, which cannot be predicted by classical methods based e.g. on the 'Kröner-Nye tensor'. After this verification we then apply our numerical implementation to a complex example: bending of a thin film in a double slip configuration, which yields most interesting results concerning the general concept of 'geometrically necessary' and 'statistically stored' dislocations. Another most important outcome is that nearly all important kinematic properties of single dislocation lines are still contained and numerically accessible within this averaged continuum description.

While we were pursuing the numerical exploration of the theory within this thesis, T. Hochrainer further developed his continuum theory towards a formulation which under certain simplifying assumptions does not require the higher order configuration space. This is extremely beneficial from point of view of computational cost and stability. A significant part of this thesis is concerned with verifying this simplified variant with the original formulation. The result is that in many physically relevant cases both theories yield very similar if not identical results.

In the third part of the thesis we tackle the problem of dislocation dynamics within the continuum description. We propose a suitable method for computing stresses based on the fact that a dislocation causes eigenstrain in an elastic continuum and demonstrate its versatility and applicability with examples.

Parts of the material used within this book has been published in the following papers:

- S. Sandfeld, M. Zaiser and T. Hochrainer, *Expansion of Quasi-Discrete Dislocation Loops in the Context of a 3D Continuum Theory of Curved Dislocations*, AIP Conference Proceedings 2009, 1168(1), 11481151.
- S. Sandfeld, M. Zaiser and T. Hochrainer, *Application of a 3D-Continuum Theory of Dislocations to Problems of Constrained Plastic Flow: Microbending of a Thin Film*, MRS Proceedings 2009, 1224-GG06-04
- S. Sandfeld, T. Hochrainer, P. Gumbsch and M. Zaiser, *Numerical Implementation of a 3D Continuum Theory of Dislocation Dynamics and Application to Microbending*, Philosophical Magazine, 2010
- S. Sandfeld, T. Hochrainer, M. Zaiser and P. Gumbsch, *Continuum modeling of dislocation plasticity: Theory, numerical implementation and validation by discrete dislocation simulations*, submitted to Journal of Materials Research as an invited paper, 2010

Preface

This work was done during my time as PhD student at the *Institute for Materials and Processes* at The University of Edinburgh, United Kingdom, in close cooperation with *izbs - Institute for Reliability of Components and Systems* at the Karlsruhe Institute of Technology (KIT), Germany, which funded more than half of my PhD project.

I would like to express my gratitude to my supervisor at the University of Edinburgh, Prof. Michael Zaiser, whose support and guidance over the past four years were invaluable to me and the project. His expertise and patience to discuss my work with me have truly broadened my understanding of materials science and physics. A very special thanks to Dr. Thomas Hochrainer. His 'Continuum Dislocation Dynamics Theory' provided a most interesting topic for my thesis and I consider it a special honor to be part of the theory's development group. Discussions with him have always been most interesting, enjoyable and enlightening. I would like to thank Prof. Peter Gumbsch (izbs) for offering the possibility of this cooperation, for very interesting and helpful discussions and for providing such an inspiring work environment.
All of them I am most grateful for teaching me science and how to put these thoughts into words. It is very precious to me that they introduced me to the scientific community and made it possible that I could present my work at international conferences and meetings.

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Thank-you to my friends and my colleagues in Edinburgh and Karlsruhe and - last but not least - to my dear family for being so very supportive and understanding all the time.

Contents

Acronyms and abbreviations

The following acronyms are used:

CCT	classical continuum theory (Kröner)
CDD	Continuum Dislocation Dynamics (Hochrainer)
sCDD	simplified version of CDD
SSD	statistically stored dislocations
GND	geometrically necessary dislocations
DDD	discrete dislocation dynamics
FE	finite element
FEM	finite element method

The following superscripts are used:

$^{\mathrm{d}}$	indicating a *discrete* object (as opposed to a continuous object)
$^{\mathrm{pl}}$	plastic
$^{\mathrm{el}}$	elastic
$^{\mathrm{s}}$	number of slip plane
$^{\mathrm{mf}}$	mean field
$^{\mathrm{y}}$	yield
$^{\mathrm{b}}$	back stress
$^{\mathrm{l}}$	line tension

The following subscripts are used to denote the point of evaluation of e.g. a function:

$_{(\boldsymbol{r},\varphi)}$	point in the configuration space
$_{(\boldsymbol{r})}$	spatial point / spatial component of a point in the configuration space
$_{(\varphi)}$	line orientation / orientational component of a point in the configuration space

Nomenclature

a	nondimensional constant in Taylor relationship
$\boldsymbol{b}$	Burgers vector
b	modulus of the Burgers vector
B	drag coefficient
$\boldsymbol{c}$	spatial curve
$\boldsymbol{C}$	lifted curve
D	nondimensional constant for back stress
$\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$	canonical unit vectors
G	shear modulus
h	film height, height of a (subvolume of a) crystal
$\boldsymbol{J}$	dislocation current
k	mean curvature
l	length of inclined slip plane (bending)
$\boldsymbol{l}$	(average) dislocation line direction
$\boldsymbol{L}$	generalised tangent
$L_{\boldsymbol{c}}$	length of a curve $\boldsymbol{c}$
M	bending moment
$\boldsymbol{n}$	(glide plane) normal vector
r, R	radius
$\boldsymbol{r}$	distance vector
$\boldsymbol{s}$	line direction of a single dislocation line
s	arc length of a curve
$\mathcal{S}$	area
$t, \Delta t$	time, discrete time step
T	line tension force
$\boldsymbol{u}$	displacement
v	scalar velocity (in general)
$\boldsymbol{v}$	vector of scalar velocity

$v_{(r,\varphi)}$	scalar velocity (in the configuration space)
w	width of a boundary layer
$\boldsymbol{V}$	generalised velocity
x, y, z	cartesian coordinates
χ	anisotropy factor for velocity
$\boldsymbol{\alpha}$	Kröner-Nye tensor
$\boldsymbol{\alpha}^{\mathrm{II}}$	dislocation density tensor of second order
$\boldsymbol{\beta}$	distortion tensor
$\boldsymbol{\varepsilon}$	strain tensor
$\epsilon_{i,j,k}$	permutation symbol
γ	plastic slip
κ	geometrically necessary dislocation density
μ	shape factor for diffusion
ν	Poisson ratio
$\boldsymbol{\nu}$	unit normal to a curve
φ	angle of line orientation
ρ	scalar dislocation density in general
ρ_{G}	geometrically necessary dislocation density
ρ_{t}	total dislocation density
$\boldsymbol{\sigma}$	stress tensor
τ	stress component (e.g. bending system)
ϑ	rotational velocity
$\mathbb{C}$	tensor of elastic moduli
$\mathcal{M}^*$	projection tensor
$\mathcal{M}$	symmetric part of the projection tensor

Calculus notations

Throughout this thesis we use the following definitions and conventions:

Vectors and tensors are denoted by bold-face letters, whereas scalar quantities are written non-bold (e.g. $\boldsymbol{\alpha}$ as opposed to α).

Partial derivatives are abbreviated as $\partial_x(\cdot) := \frac{\partial(\cdot)}{\partial x}$, ∇ denotes the gradient operator and the divergence of a vector (tensor) field is written as div, curl denotes the curl-operator. Second partial derivatives are abbreviated by a double subscript $\partial_{xy}(\cdot) := \frac{\partial}{\partial x}\frac{\partial(\cdot)}{\partial y}$.

The vector product is denoted by $\times$. For double indices we assume the summation convention, if not stated otherwise. In $\boldsymbol{c} = \boldsymbol{a} \otimes \boldsymbol{b}$ the tensor product is denoted by $\otimes$; this operation reads for Cartesian coordinates in index notation $c_{ij} = a_i b_j$.

The symmetric part of a tensor $\boldsymbol{a}$ is denoted by $\operatorname{Sym} \boldsymbol{a} := \frac{1}{2}\left(\boldsymbol{a} + \boldsymbol{a}^T\right)$.

We denote the twofold derivative in direction of the vector $\boldsymbol{L}$ by $\nabla^2_{\boldsymbol{L}}(v)$, where v is a scalar.