8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineeering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

3D-Continuum Theory of Dislocations: Numerical Implementation and Application

*** S. Sandfeld[1,3], T. Hochrainer[1,2] and M. Zaiser[3]**

[1] Universität Karlsruhe,
Institut für die Zuverlässigkeit von Bauteilen und Systemen,
Kaiserstr. 12,
76131 Karlsruhe, Germany
stefan.sandfeld@kit.edu
www.izbs.uni-karlsruhe.de

[2] Fraunhofer Institut für Werkstoffmechanik IWM
Wöhlerstr. 11,
79108 Freiburg, Germany
thomas.hochrainer@iwm.fhg.de
http://www.iwm.fhg.de

[3] The University of Edinburgh, Centre for Materials Science and Engineering,
King's Buildings
Edinburgh, United Kingdon
m.zaiser@ed.ac.uk,
http://www.see.ed.ac.uk

Key Words: *continuum theory of dislocations, crystal plasticity, numerical implementation*

ABSTRACT

The growing demand for physically motivated continuum theories of plasticity led to an increased effort on continuum descriptions based on dislocations. For simplified systems of straight parallel edge dislocations in a single slip configuration a quasi two-dimensional theory is available, derived by methods of statistical mechanics for interacting particle systems [1].

However, earlier attempts to transfer this method to three-dimensional systems of curved dislocations failed. This was due to the inability of the classical dislocation density measures to reflect all dislocations as line like objects. The reason is that the Kröner tensor α [2], as a measure for geometrically necessary dislocations (GND) comprises only a fraction of all dislocations, while the scalar density of statistically stored dislocations (SSD) contains no directional information.

This deficiency was remedied by a recently introduced extended continuum theory of dislocations [3]. This theory utilizes a generalized definition of the dislocation density tensor, the so-called dislocation density tensor of second order, α^{II}. Within this tensor all dislocations appear as line like objects; the distinction between GND and SSD becomes dispensable. Therefore this theory allows for a *meaningful* averaging process.

We study the extended continuum theory for the 2-dimensional special case of a single glide system. For this special case the tensorial evolution equation of the dislocation density tensor α^{II} can be reformulated into two evolution equations for the scalar-valued fields *scalar dislocation density* ρ and *curvature* k. These equations were numerically implemented by use of a finite difference scheme for the spatial derivatives and a forward Euler time integration scheme.

We numerically validate the theory by showing that these continuum evolution equations can handle the kinematic evolution of discrete dislocations. The constituents of these evolution equations and their implications for the numerical implementation will be explored by numerical examples. We show, that our method can treat various kinds of dislocation distributions - density fields as well as quasi-discrete dislocations.

We derive the set-up for the numerical treatment of impenetrable boundary conditions. The effect of dislocation pile-ups at impenetrable boundaries is studied and compared to alternative approaches (e.g. [4]).

Furthermore, we show the necessary steps for embedding the evolution equations (on the meso-scale) into a crystal plasticity context (on the micro-scale). This allows for computation of stress field evolution and dislocation patterning, e.g. for composite materials as shown in [5] and [6].

REFERENCES

[1] M. Zaiser, M.C. Miguel, I.Groma. “Statistical dynamics of dislocation systems: The influence of dislocation-dislocation correlations”, *Phys. Rev. B*, Vol. **64**, 2001.

[2] E. Kröner. “Kontinuumstheorie der Versetzungen und Eigenspannungen” , *Springer Verlag, Berlin*, 1958.

[3] T. Hochrainer, M. Zaiser, P. Gumbsch. “A three-dimensional continuum theory of dislocation systems: kinematics and mean-field formulation”, *Phil. Mag.*, Vol. **87**, 2007.

[4] R. Sedláček, J. Kratochvíl, E. Werner, ”The importance of being curved: bowing dislocations in a continuum description”, *Phil. Mag.*, Vol. **83**, 2003.

[5] S. Yefimov, I. Groma, E. Van der Giessen, ”A comparison of a statistical-mechanics based plasticity model with discrete dislocation plasticity calculations”, *J. Mech. Phys. Solids*, Vol. **52**, 2003.

[6] H.H.M. Cleveringa, E. Van der Giessen,A. Needleman, ”Comparison of discrete dislocation and continuum plasticity predictions for a composite material”, *Acta mater.*, Vol. **45**, 1995.