11th. World Congress on Computational Mechanics (WCCM2014)
5th. European Conference on Computational Mechanics (ECCM V)
6th. European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

COMPUTATIONAL MECHANICS OF DISLOCATIONS

STEVEN FITZGERALD[*†], EDMUND TARLETON[†] AND DANIEL BALINT[‡]

[*] Culham Centre for Fusion Energy, Culham Science Centre, Abingdon OX14 5AX, UK
steven.fitzgerald@materials.ox.ac.uk

[†] Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK
edmund.tarleton@materials.ox.ac.uk

[‡] Department of Mechanical Engineering, Imperial College, London SW7 2AZ, UK
d.balint@imperial.ac.uk

Key words: Dislocations, defects, mechanical properties.

ABSTRACT

The motion of dislocations and other defects governs the mechanical properties of crystalline materials, and can also strongly influence their electronic, acoustic and optical behaviour. Though first proposed almost 100 years ago, and observed in the microscope in the 1950s, the computer simulation of representatively large ensembles of dislocations has only relatively recently been attempted. Approaches to dislocation modelling run the gamut of solid simulation techniques and lengthscales, from electronic structure calculations [1], through molecular dynamics (MD) [2], mesoscale discrete dislocation dynamics (DDD) [3] simulations to macroscopic crystal plasticity (CP) and finite element analysis (FEM) [4]. In recent years, innovative approaches such as phase field models [5] and level sets [6] have been applied to computational defect mechanics. As such, it represents an archetypal example of multiscale modelling. Furthermore, advances in microscopy and micromechanical testing techniques allow the probing of ever-smaller lengthscales, highlighting the role computer simulations have to play in bridging the gap in scales between the fundamental microscopic theories of material behaviour and the lengthscales accessible to experiment and relevant to industrial applications.

This minisymposium aims to bring together international experts in dislocation mechanics from across the spectrum of modelling techniques, length- and time-scales. Particularly welcome are papers which aim to bridge two or more complementary approaches and scales.

Submissions are sought in areas including, but not limited to:

- Fundamentals and applications of DDD simulations
- Coarse-graining and scale-bridging between MD, DDD and CP/FEM
- Statistical and stochastic simulation techniques and applications
- Modelling of dislocations and plasticity at small scales
- Nonlinear and non-equilibrium dynamics of defects
- Dynamics of defects under extreme conditions e.g. shock loading, high temperatures, irradiation.

SELECTED REFERENCES

[1] **"**Core structure and Peierls potential of screw dislocations in α-Fe from first principles: cluster versus dipole approaches", L. Ventelon and F, Willaime, *J. Comp.-Aided Mater. Des.* **14** 85-94 (2007);

[2] "Strengthening due to coherent Cr precipitates in Fe--Cr alloys: Atomistic simulations and theoretical models," D. Ternetyev *et al, Act;a Mat.* **56** (13) 3229-3235 (2008);

[3] "Enabling strain hardening simulations with dislocation dynamics", A. Arsenlis *et al*, *Mod. Simul. Mater. Sci. Eng.* **15** (6)553 (2007);

[4] "Size and boundary effects in discrete dislocation dynamics: coupling with continuum finite element", Yasin *et al, Mat. Sci. Eng.* **309** 294-299 (2001);

[5] **"**Nanoscale phase field microelasticity theory of dislocations: model and 3D simulations", Wang *et al*, *Acta Mat.* **49** (10) 1847-1857 (2001);

[6] **"**A level set method for dislocation dynamics", Xiang *et al, Acta Mat.* **51** (18) 5499-5518 (2003).