

# DISLOCATIONS 2008

*An International Conference on the Fundamentals of Plastic Deformation  
October 13-17, 2008      Hong Kong*



*Book of Abstracts*

## Sponsors:



The Croucher Foundation



National Science Foundation



The University of Hong Kong



The University of Tokyo



Stanford University

## Executive Committee:

D. Barnett (Stanford, USA)  
V. V. Bulatov (LLNL, USA)  
D. Caillard (CEMES, France)  
B. Devincere (LEM, France)  
L. Kubin (LEM, France)  
E. Kuramoto (Kyushu Univ., Japan)  
H. Mughrabi (Erlangen Univ., Germany)  
A. Needleman (Brown Univ., USA)  
P. Veyssiere (LEM, France)  
S. Roberts (Oxford Univ., UK)  
R. Selinger (CUA, USA)  
M. Tang (LLNL, USA)

## Scientific Committee:

A. S. Argon (MIT, USA)  
E. Arzt (MPI Stuttgart, Germany)  
D. Bacon (Liverpool Univ., UK)  
D. Banerjee (DMRL, India)  
P. Gumbsch (IWM Fraunhofer, Germany)  
D. Juul-Jensen (Riso, Denmark)  
P. H<sub>2</sub>ner (JRC, Netherland)  
R. Hoagland (LANL, USA)  
L. Levin (NIST, USA)  
D. Rodney (GPM2, France)  
C. Teodosiu (Paris Nord Univ., France)

## Organizing Committee:

A. H. W. Ngan (HKU, China)  
W. Cai (Stanford, USA)  
K. Edagawa (Univ. Tokyo, Japan)

# Table of Contents

## Oral Presentations:

A new model for dynamic recovery in stage III deformation of fcc metals (invited paper) – <i>A.S. Argon</i>	1
Dislocation climb plasticity: modeling and comparison with the high-temperature mechanical properties of quasicrystalline AlPdMn, and superalloys – <i>Frederic Momprou and <u>Daniel Caillard</u></i>	2
Introducing dislocation climb by bulk diffusion in discrete dislocation dynamics simulations – <i><u>Dan Mordehai</u>, Emmanuel Clouet, Marc Fivel and Marc Verdier</i>	3
Mechanistic insights for modeling dislocation climb – <i><u>Timothy Lau</u>, Mukul Kabir, Krystyn Van Vliet and Sydney Yip</i>	4
In situ study of the evolution of dislocation structures during strain path changes – <i><u>C. Wejdemann</u>, W. Pantleon, U. Lienert and H.F. Poulsen</i>	5
Crackling plasticity (invited paper) – <i>Jérôme Weiss</i>	6
Dislocation dynamics, mean free path and slip avalanches in fcc crystals – <i><u>Benoit Devincere</u>, Ladislav P. Kubin and Thierry Hoc</i>	7
Statistical characterization of dislocation systems with dislocation dynamics simulation – <i><u>Ferenc F. Csikor</u> and Istvan Groma</i>	8
Topology and transport in driven vortex lattices – <i><u>Paolo Moretti</u> and M. Carmen Miguel</i>	9
Evolution of Dislocation Patterns in FCC Metals – <i><u>P. Landau</u>, R.Z. Shneck, G. Makov and A. Venkert</i>	10
2 - dimensional dislocation dynamics models of the brittle-ductile transition in body-centred cubic metals (invited paper) – <i>E. Tarleton and <u>S.G. Roberts</u></i>	11
Dislocation dynamical modelling of the ductile-brittle-transition – <i><u>Thomas Hennecke</u> and Peter Hähner</i>	12
Research in mechanics and materials – <i>Ken P. Chong</i>	13
Irreversible thermodynamics modeling of plastic deformation over wide ranges of strain rates – <i><u>Mingxin Huang</u>, Pedro E.J. Rivera-Diaz-del-Castillo, Olivier Bouaziz and Sybrand van der Zwaag</i>	14

In-situ deformation experiments: insights in small scale plasticity (invited paper) – <i>G. Dehm</i>	15
Determination of Geometrically Necessary Dislocations Distributions using Electron Backscatter Diffraction – <i>Angus J Wilkinson</i>	16
Dislocation source-controlled plasticity in fcc micropillars: recent experiments and modeling using the line tension approximation (invited paper) – <i>William D. Nix, Seok-Woo Lee, Christopher Weinberger and Wei Cai</i>	17
Smaller is stronger: a view obtained by in-situ Laue diffraction – <i>R. Maaß, J. Zimmermann, S. Van Petegem, H. Van Swygenhoven</i>	18
Statistical Description of the Intermittent Plasticity and Creep of Micron-sized Crystal Pillars – <i>A.H.W. Ngan and K.S. Ng</i>	19
Discrete dislocation dynamics study of the mechanical properties of micro-samples – <i>J. Senger, D. Weygand, P. Gumbsch and O. Kraft</i>	20
Dislocation dynamics and plasticity in FCC and BCC single crystal micro-pillars – <i>Christopher R. Weinberger and Wei Cai</i>	21
<i>In-situ</i> nanocompression of gum metal pillars – <i>E. Withey, J. Ye, A. Minor, S. Kuramoto, D.C. Chrzan and J.W. Morris, Jr.</i>	22
Athermal mechanisms of size-dependent crystal flow gleaned from three-dimensional discrete dislocation simulations (invited paper) – <i>S.I. Rao, D.M. Dimiduk, T.A. Parthasarathy, M.D. Uchic, M. Tang and C. Woodward</i>	23
Pillar plasticity: 2.5D dislocation dynamics simulations – <i>A. Amine Benzerga and P.J. Guruprasad</i>	24
In situ investigation of nano-scale plasticity in FCC and BCC crystals via homogeneous deformation of nano-pillars – <i>J.R. Greer, Ju-Young Kim and Steffen Brinckmann</i>	25
Dislocation source activation approach to explain size effects on plasticity in ultra thin metallic films of different microstructure – <i>Patric A. Gruber, Rudolf Baumbusch, Eduard Arzt, Ralph Spolenak and O. Kraft</i>	26
Extended dislocations and dislocation reactions in L1 <sub>2</sub> ordered superalloys – <i>R.E. Voskoboynikov and C.M.F. Rae</i>	27
How metallic thin films on substrate accommodate or resist plastic deformation: the contribution on <i>in situ</i> TEM experiments (invited paper) – <i>M. Legros</i>	28
Brittle and ductile failure of Si nanowires in tension, torsion and bending – <i>Wei Cai, Keonwook Kang, Will Fong, Erich Elsen and Christopher R. Weinberger</i>	29

Plasticity of nanocomposite wires during in-situ tensile tests under X-rays: size effect, Bauschinger effect and dislocation storage – <u>L. Thilly</u> , <u>P.O. Renault</u> , <u>V. Vidal</u> , <u>S. Van Petegem</u> , <u>H. Van Swygenhoven</u> and <u>F. Lecouturier</u>	30
Electrical properties of dislocations in GaN – <u>Yasushi Kamimura</u> , <u>Takashi Yokoyama</u> , <u>Hirokazu Oiwa</u> , <u>Keiichi Edagawa</u> and <u>Ichiro Yonenaga</u>	31
Dislocation self-organization in fcc metals deformed in single slip: the underlying microscopic manoeuvres (invited paper) – <u>Patrick Veyssière</u> , <u>Hao Wang</u> and <u>Dongsheng Xu</u>	32
Suzuki segregation – <u>B.G. Mendis</u> , <u>I.P. Jones</u> and <u>R.E. Smallman</u>	33
Strain localization in post-irradiated metals: TEM observations, molecular dynamics and dislocation dynamics analysis – <u>T. Nogaret</u> , <u>C. Robertson</u> , <u>M. Fivel</u> and <u>D. Rodney</u>	34
Suppressing dislocation glide to achieve ideal strength – <u>J.W. Morris, Jr.</u> , <u>E. Withey</u> , <u>T. Li</u> and <u>D.C. Chyrzan</u>	35
Bridging atomic to continuum scale through thermodynamic analysis of molecular dynamics simulations: case of dislocation-void interaction – <u>Ghiath Monnet</u>	36
Dislocation Observation in Protein Crystals by Synchrotron X-ray Topography – <u>Masaru Tachibana</u> and <u>Kenichi Kojima</u>	37
Atomic-scale modeling of dislocation interaction with localized obstacle (invited paper) – <u>Yu. N. Osetsky</u> and <u>D.J. Bacon</u>	38
Quantification of Solute Segregation at Dislocations – <u>M.K. Miller</u>	39
Solute and dislocation junction interactions – <u>Q. Chen</u> , <u>X-Y Liu</u> and <u>S.B. Biner</u>	40
Atomistic simulations of dislocation-obstacle interactions – <u>Brian D. Wirth</u> , <u>Jae-Hyeok Shim</u> and <u>Hyon-Jee Lee</u>	41
Non-Schmid plastic behavior and differences in slip activity in molybdenum and tungsten resulting from the core structure of screw dislocations – <u>Roman Groger</u> and <u>Vaclav Vitek</u>	42
Dislocation Atomic Structures and Properties in Sapphire (invited paper) – <u>Yuichi Ikuhara</u>	43
Scaling constraints associated to plastic flow in nanograined polycrystals – <u>G. Saada</u>	44
On the core structure of dislocations in elemental semiconductors at high stresses – <u>J. Rabier</u> , <u>J.L. Demenet</u> , <u>D. Eyidi</u> and <u>A.A. Shiryaev</u>	45
Dislocation impurity interaction in Si – <u>Ichiro Yonenaga</u> , <u>Toshinori Taishi</u> and <u>Yutaka Ohno</u>	46

Interface and surface controlled plasticity in nanostructured metals (invited paper) – <i>Ju Li</i>	47
Dislocation dynamics and the plasticity of single crystals – <i>Ladislav Kubin, Thierry Hoc and B. Devincre</i>	48
Rigorous homogenization results for dislocation dynamics – <i>Regis Monneau</i>	49
Modelling slip transfer across a tilt grain boundary in 2D discrete dislocation plasticity – <i>Ranjeet Kumar, Ferenc Szekeley, Lucia Nicola and Erik Van der Giessen</i>	50
Atomistically-informed dislocation dynamics simulations of dislocation-defect interactions in fcc crystals – <i>E. Martinez, J. Marian, A. Arsenlis, M. Victoria and J.M. Perlado</i>	51
The effect of the $\alpha$ - $\gamma$ phase transition on dislocations in ferromagnetic bcc iron – <i>S. L. Dudarev, R. Bullough, and P. M. Derlet</i>	52
Subgrains observed by high energy x-ray diffraction during in-situ loading (invited paper) – <i>W. Pantleon, U. Lienert, C. Wejdemann, B. Jakobsen and H.F. Poulsen</i>	53
Algorithm for activated state trajectory – <i>Sidney Yip, Akihiro Kushima, Timothy Lau, Xi Lin, and Ju Li</i>	54
Interfaces within discrete dislocation dynamics simulations – <i>Katerina E. Aifantis and Michael Zaiser</i>	55
A generalized Peierls-Nabarro model for curved dislocations – <i>Yang Xiang, He Wei, Pingbing Ming and Weinan E</i>	56
Non-singular dislocation fields – <i>Elias C. Aifantis</i>	57
Viscoplasticity and plastic heterogeneities in ice single crystals loaded in torsion: a comparison between experiments and discrete dislocation dynamics simulations (invited paper) – <i>Juliette Chevy, Marc C. Fivel and Paul Duval</i>	58
Discrete dislocation plasticity modeling of polycrystal plasticity – <i>Alan Needleman and Erik Van der Giessen</i>	59
Migration of intergranular boundaries as a response of dislocation arrays to applied stress – <i>Dmitri A. Molodov, Tatiana Gorkaya and Gunter Gottstein</i>	60
Ultrasound as a probe of plasticity? The interaction of elastic waves with dislocations – <i>Agnes Naurel, Vincent Pagneux, Felipe Barra and Fernando Lund</i>	61

Perfect dislocation mobility in silicon: theoretical study of kinks formation and migration – <i>Laurent Pizzagalli, Andreas Pedersen, Andri Arnaldsson, Hannes Jonsson and Pierre Beauchamp</i>	62
Dislocation patterning and formation of Omega phase in shock-loaded tantalum – <i>Luke Hsiung</i>	63
Origin of dynamic strain aging in metals: solute aging of both mobile and forest dislocations (invited paper) – <i>M. Soare and W. A. Curtin</i>	64
Stress functions for dislocation loops in anisotropic crystals – <i>Kazuhito Ohsawa, Masatoshi Yagi, Hirokazu Koizumi and Eiichi Kuramoto</i>	65
Grand scaling of the temperature dependence of the strength of crystals governed by the Peierls mechanism – <i>S. Takeuchi and T. Suzuki</i>	66
3D-continuum theory of dislocations: numerical implementation and application – <i>S. Sandfeld, T. Hochrainer, M. Zaiser and P. Gumbsch</i>	67
Energy flow around a moving dislocation – <i>H. Koizumi and H. O. K. Kirchner</i>	68

**Poster Presentations:**

3-dimensional dislocation dynamics modelling of hardening effects of radiation damage in iron – <i>R. Novoksharov and S.G. Roberts</i>	69
3D - stress analysis during crack-crazing patterns interactions in a polystyrene material – <i>M. Chabaat and H. Seddiki</i>	70
Stress analysis during the interaction between dislocations and a main crack: case of a bi-material – <i>M. Chabaat and H. Hamli Ben Zahar</i>	71
Breakdown of self-similar hardening behavior in Au nanopillar microplasticity – <i>Jaime Marian and Jaroslaw Knap</i>	72
New in situ experiments in Fe at low temperature – <i>Daniel Caillard</i>	73
Nanoindentation studies of dislocation-grain boundary interactions – <i>Ben Britton, David Randman, and Angus J Wilkinson</i>	74
Investigation of dislocation mobility in small periodic cells using the Nudged Elastic Band method: effect of a confinement pressure – <i>Laurent Pizzagalli, Hannes Jonsson and Pierre Beauchamp</i>	75

Atomistic calculations of the formation, stability and mobility of a non-dissociated 60° dislocation in silicon – <i>Julien Godet, Sandrine Brochard, Tristan Albaret and <u>Laurent Pizzagalli</u></i>	76
Matching asymptotic expansion in modeling of edge dislocation pile-ups – <i><u>R.E. Voskoboynikov</u>, S.J. Chapman and J.R. Ockendon</i>	77
Evaluation of recovery kinetics of AA3103 using stress relaxation tests – <i><u>Sheila Bhaumik</u> and Gunter Gottstein</i>	78
Peierls-Nabarro model and kink pair nucleation in MgO – <i><u>Philippe Carrez</u> and Patrick Cordier</i>	79
Dislocation modeling of perovskites using the Peierls-Nabarro model – <i>Denise Ferré, <u>Patrick Cordier</u> and <u>Philippe Carrez</u></i>	80
Mechanical behaviour and deformation mechanism of a niobium alloy with different carbon content – <i><u>Rengen Ding</u> and Ian P Jones</i>	81
Some correlations between slip band emergence and dislocation pattern – <i>Corrine Huvier, Egle Conforto, G. Girardin, D. Delafosse and <u>Xavier Feaugas</u></i>	82
Atomistic simulation of He bubble in Fe as obstacle to dislocation – <i><u>S.M. Hafez Haghghat</u>, G. Lucas and R. Schäublin</i>	83
Study of dislocation nucleation activation from surface step by atomistic calculations – <i><u>P. Hirel</u>, J. Godet, S. Brochard and L. Pizzagalli</i>	84
Incorporating nonlinear elasticity into a 2D theory of dislocations – <i><u>Peter Dusan Ispanovity</u> and Istvan Groma</i>	85
Dislocation structure evolution of Al alloy deformed at a high strain rate – <i><u>Hyung-Ha Jin</u>, Chansun Shin and Yoo-Jin Oh</i>	86
Plasticity of miniaturized tension and compression samples – <i><u>D. Kiener</u>, J. Keckes, R. Pippan and G. Dehm</i>	87
Deformation substructure formation – <i><u>Jan Kratochvil</u>, Martin Kružík1 and Radan Sedláček</i>	88
Grain boundary sliding induced by lattice dislocation activity during ambient temperature creep in h.c.p. metals – <i><u>Tetsuya Matsunaga</u>, Tatsuya Kameyama and Eiichi Sato</i>	89
In-plane work hardening effect of dislocation loops in particle strengthened alloys – <i>Volker Mohles</i>	90

The indentation size effect and the arrangement of geometrically necessary dislocations – <u>C. Motz</u> , <i>M. Rester, H. Kreuzer and R. Pippan</i>	91
Characterisation of plastic zones around crack-tips in BCC metals using electron backscattered diffraction – <u>J.D. Murphy</u> , <i>T.D. Joseph, E. Tarleton, A.J. Wilkinson and S.G. Roberts</i>	92
Structure and behavior of basal dislocations in sapphire – <u>Atsutomu Nakamura</u> , <i>Eita Tochigi, Naoya Shibata, Takahisa Yamamoto and Yuichi Ikuhara</i>	93
Studies of plastic deformation using phenomenological mesoscale field dislocation mechanics – <i>Satya Varadhan, Saurabh Puri, Armand Beaudoin, Amit Acharya and Claude Fressengeas</i>	94
Dislocation transport in crystal plasticity – <u>C. Fressengeas</u> , <i>A.J. Beaudoin, D. Entemeyer, T. Lebedkina, M. Lebyodkin and V. Taupin</i>	95
The Orowan mechanism and its composition with forest hardening in ferrite: a DD simulation study – <u>Sylvain Queyreau</u> , <i>Ghiath Monnet and Benoit Devincere</i>	96
Deformation luminescence of X-irradiated KCl:Eu <sup>2+</sup> by bending test – <u>S. Nakamura</u> , <i>K. Kawaguchi and T. Ohgaku</i>	97
Interaction between dislocation and divalent impurities in KBr single crystals – <u>T. Ohgaku</u> and <i>T. Matsunaga</i>	98
Optical properties of dislocations in wurtzite ZnO single-crystals – <u>Y. Ohno</u> , <i>H. Koizumi, T. Taishi, I. Yonenaga, K. Fujii, H. Goto, and T. Yao</i>	99
Solid solution hardening in faced centred binary alloys – <u>S. Patinet</u> and <i>L. Proville</i>	100
Anomalous mobility of dislocation kink solitons in disordered solid solutions – <i>B. V. Petukhov</i>	101
Ab-initio calculations of screw dislocations in tungsten and tungsten-Re alloys – <u>Lorenz Romaner</u> , <i>Claudia Ambrosch-Draxl and Reinhard Pippan</i>	102
Dynamic dislocation-defect analysis: forest dislocations, solutes, clusters and transition phases – <i>S. Saimoto</i>	103
Discrete transformation-dislocation model – <u>Jingyi Shi</u> , <i>Sergio Turteltaub and Eric Van der Giessen</i>	104
HRTEM observation of displacement fields around dislocations in quasicrystals – <u>Yeong-Gi So</u> and <i>Keiichi Edagawa</i>	105

Dislocation core interaction in low-angle grain boundaries of alumina – <i>E. Tochigi, N. Shibata, A. Nakamura, T. Yamamoto and Y. Ikuhara</i>	106
Dislocation based modeling of plasticity in superalloy single crystals: hybrid DD-FE simulations – <i>A. Vattré, A. Roos and B. Devincré</i>	107
Core structure, Peierls potential and kinks of screw dislocations in $\alpha$ -Fe from first principles – <i>Lisa Ventelon, François Willaime and Emmanuel Clouet</i>	108
Formation of point defect by dislocation reaction in some metals and intermetallic compounds – <i>Dongsheng Xu, Hao Wang and Rui Yang</i>	109
Deformation defects: from dislocations to plasticity localization waves – <i>Lev B. Zuev and Svetlana A. Barannikova</i>	110
Plastic deformation of silicon wafer to shaped-crystal – <i>Ichiro Yonenaga, Kozo Fujiwara, Koji Okuda and Kazuo Nakajima</i>	111
Resolving the geometrically necessary dislocation content in zircon by conventional EBSD – <i>Wolfgang Pantleon, Steven M. Reddy and Nicholas E. Timms</i>	112
Dislocation activity within nanocrystalline metals: a molecular dynamics study – <i>C. Brandl, E. Bitzek, P. M. Derlet and H. Van Swygenhoven</i>	113
Phase field modelling of stacking fault shear in nickel base superalloys – <i>V. A. Vorontsov and C. M. F. Rae</i>	114
Interaction of an edge dislocation with $\frac{1}{2}\langle 111 \rangle$ and $\langle 100 \rangle$ dislocation loops in $\alpha$ -Fe: an atomistic study – <i>D. Terentyev, D.J. Bacon and Yu.N. Osetsky</i>	115
Strengthening due to Cr precipitates in Fe-Cr alloys : theory vs. atomistic simulations – <i>D. Terentyev, L. Malerba and G. Bonny</i>	116
ECCI observation of dislocation structures around fatigue cracks in ferritic stainless steel single crystals – <i>T. Taniguchi, Y. Kaneko and S. Hashimoto</i>	117
A dislocation-based approach to identify fracture process – <i>Y. Kaneko, Y. Honda and S. Hashimoto</i>	118
Hardness and deformation mechanisms of $Ti_3SnC_2$ studied by nanoindentation and AFM – <i>Christophe Tromas, Nadia Ouabadi, Véronique Gauthier, Michel Jaouen, Patrick Villechaise and Sylvain Dubois</i>	119
Pop-in phenomenon and nucleation of dislocations during nanoindentation in MgO – <i>Christophe Tromas, Alex Montagne, Valérie Audurier and Jacques Woignard</i>	120

Direct evidence for the key role of dislocation mechanisms in work hardening of single up to nanostructured crystals under internal friction, fatigue and shock loadings – <i>Valery P. Kisel</i>	121
New evidences for the deformation origin of insulator-metal-superconductor, normal-superfluid transitions – <i>V.P. Kisel</i>	122
The same key mechanisms of serrated flow of crystals along the deformation curves in the range from $\varepsilon \sim 10^{-8}$ to $\varepsilon \leq 10^3$ – <i>Valery P. Kisel</i>	123
Plastic deformation mechanisms of MAX phase $\text{Ti}_4\text{AlN}_3$ and the core structure of dislocations – <i>Ludovic Thilly, Anne Joulain and Jacques Rabier</i>	124

**A new model for dynamic recovery in Stage III deformation of FCC metals**

A. S. Argon  
Massachusetts Institute of Technology  
Cambridge MA 02139

Since the early researches on the strain hardening of FCC metals in the 50s by Seeger and others who followed, it has been generally accepted that dynamic recovery in Stage III deformation of FCC metals is controlled by massive cross slip of screw dislocations, circumventing linear Lomer-Cottrell (LC) dislocation barriers and results in decreasing strain hardening rates. Apart from fragmentation of slip bands and the dependence of  $\tau_{III}$ , on stacking fault energy, which can both be explained differently, this proposition is quite inconsistent with the cellular dislocation microstructure that develops in Stage III hardening, and can not provide a rational explanation of its self similar reduction in scale with increasing plastic resistance.

In a proposed new mechanism dynamic recovery results from the systematic removal of LC locks in cell walls under the repeated impingement of dislocation fluxes that, in turn, trigger associated collapse events in much of the pinned redundant cell wall dislocation microstructure. This then provides the required kinematic degrees of freedom for displacement of cell walls and permits the flow-noise-induced cell refinement process of Haehner and Zeiser, to develop unhindered. The model correctly predicts the onset of dynamic recovery at  $\tau_{III}$ , its dependence on temperature and stacking fault energy, as well as the temperature and stress dependence of the decreasing strain hardening rate of Stage III, referred to as the Voce Law.

## **Dislocation climb plasticity: modelling and comparison with the high-temperature mechanical properties of quasicrystalline AlPdMn, and superalloys**

Frederic Momprou and Daniel Caillard  
CEMES-CNRS, BP 4347, 31055 Toulouse Cedex, France.

We propose a model which fully accounts for several unexplained aspects of the mechanical properties of icosahedral AlPdMn, published in the literature. This model is based on *post mortem* and *in situ* TEM observations of two dislocation families moving by pure climb and exchanging vacancies. It provides the first direct evidence of the chemical (or osmotic) force induced by an out-of-equilibrium vacancy concentration. It relies on the following properties which can be considered as the signature of pure climb plasticity:

- a high strain-hardening at yield, due to a strong decrease of the concentration of vacancies consumed by climbing dislocations,
- a steady-state flow stress twice higher than the elastic limit, which is accounted for by the equilibrium value of the chemical stress,
- two-stages relaxation curves defining strain-rate sensitivities in a ratio of 2, which are a direct consequence of the complex relaxation of the chemical stress.

The true stress-dependence of the dislocation climb velocity, which has been determined accordingly, is different from the linear dependence given by classical models valid at low stress. It is however in a fair agreement with the model of Hirth and Lothe, which describes the nucleation of jog pairs on straight dislocation segments observed in TEM. The best fit is obtained for a jog height of about 1nm, i.e. of the order of the average distance between cluster rows.

These conclusions may be transposed to crystals deformed under specific conditions favouring pure climb deformation. The high-temperature creep of superalloys, in which climbing dislocations also exchange vacancies, will be treated as an example.

## Introducing Dislocation Climb by Bulk Diffusion in Discrete Dislocation Dynamics Simulations

Dan Mordehai<sup>1,2</sup>, Emmanuel Clouet<sup>1,3</sup>, Marc Fivel<sup>4</sup> and Marc Verdier<sup>4</sup>

<sup>1</sup> SRMP, CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France.

<sup>2</sup> Department of Materials Engineering, Technion-Israel Institute of Technology, 32000 Haifa, Israel.

<sup>3</sup> LMPGM, Université Lille, 59655 Villeneuve d'Ascq Cedex, France.

<sup>4</sup> SIMaP, Grenoble INP, CNRS/UJF, BP 75, 38402 St. Martin d'Heres, France.

One of the powerful computational tools to study dislocation microstructure and plasticity at the mesoscopic scale is Dislocation Dynamics simulations, in which dislocations are treated as elastic entities. In this talk, we present a method to incorporate dislocation climb by bulk diffusion in Dislocation Dynamics simulations, by coupling this simulation technique with the diffusion theory of vacancies. We adapt the method to a 3-dimensional Discrete Dislocation Dynamics (DDD) simulation, in which each dislocation is represented by pure edge and screw dislocation segments. We firstly discuss the case in which the interaction between the flux fields of climbing segments is omitted. The calculation is demonstrated by simulating the activation of a Bardeen-Herring climb source upon the application of an external stress or under vacancy supersaturation, as well as isolated dislocation prismatic loops shrinkage and expansion. The model is then extended to allow climb in bulk materials, where dislocations are sources of vacancies, by considering simple interaction between the segments' flux fields. Subsequently, the model is shown to reproduce the coarsening of dislocation loops in annealed bulk. We observe in our simulations that large dislocation loops expand on the expense of smaller ones. Medium size loops are found to translate from expansion to shrinkage, as the vacancy supersaturation is relieved along the calculation. The processes observed in our simulations agree with experimental observations in fcc metals.

## **Mechanistic Insights for Modeling Dislocation Climb**

Timothy Lau, Mukul Kabir, Krystyn Van Vliet, and Sidney Yip  
Department of Materials Science and Engineering and Department of Nuclear Science and Engineering, MIT, Cambridge, MA 02139

The interaction between dislocation climb and glide is a central issue in understanding creep. While there are atomistic methods to treat glide, the study of climb is still a challenge. The long time scale nature of dislocation climb mandates that modeling such phenomenon requires coarse graining the atomistic details of one or more vacancies binding to dislocation core. We use an empirical interatomic potential for BCC Fe<sup>1</sup> to obtain atomistic details of vacancy diffusion near a (110)<111> dislocation core, the intention being to extract mechanisms that can be fed into kinetic Monte Carlo simulations of climb. We will present results on binding and migration activation of the single vacancy as a function of distance from the core, along with evidence showing the adparticle nature of binding of additional vacancies. We then build upon this understanding to discuss results on the migration energetics of the additional vacancies relative to that of the single vacancy migration. From these results we obtain a general set of self-consistent observations on vacancy-core binding, and discuss their applicability in a kinetic Monte Carlo simulation framework.

We gratefully acknowledge financial support from SKF Global, Inc. and from the US National Defense Science and Engineering Graduate program (T. T. L.).

**Preference:** Oral Presentation

**Presenter:** Timothy Lau

<sup>1</sup> T. T. Lau, C. J. Först, X. Lin, et al., Physical Review Letters **98**, 215501 (2007).

[NOTE: I would like this abstract to be considered for the travel fellowship.]

## **In situ study of the evolution of dislocation structures during strain path changes**

C. Wejdemann<sup>1</sup>, W. Pantleon<sup>1</sup>, U. Lienert<sup>2</sup>, H. F. Poulsen<sup>1</sup>

<sup>1</sup> Center for Fundamental Research: Metal Structures in Four Dimensions,  
Materials Research Department, Risø DTU, Denmark

<sup>2</sup> APS, Argonne National Laboratory, USA

During plastic deformation of metals, such as copper, dislocations are produced, and as the dislocation density increases their arrangement becomes markedly heterogeneous. A structure is formed, consisting of almost dislocation free regions separated by dislocation rich boundaries. This structure changes as the deformation proceeds leading to progressively smaller boundary spacings.

At the APS synchrotron we have set up a novel X-ray diffraction technique, which combines an angular resolution of 5 millidegrees with fast three-dimensional reciprocal space mapping. This allows us to see reflections from deeply embedded dislocation free volumes and study the evolution of dislocation structures in polycrystalline copper samples during strain path changes. During a strain path change, the main axes of the deformation are altered, and the dislocation structure established during pre-deformation may become unstable and be replaced by a new structure characteristic of the new deformation conditions.

The strain path changes considered are tension-tension sequences. Polycrystalline copper sheets are pre-deformed in tension to 5% strain and tensile specimen are cut with varying angles between the first and second loading axis. The second tensile deformation up to additional 5% strain is performed in situ while mapping a selected X-ray reflection of one particular bulk grain with high angular resolution. In this way, we are able to establish a systematic correlation between changes in the dislocation structure and the degree of the strain path change.

**Preference:** Oral presentation

**Presenter:** Christian Wejdemann

# Crackling Plasticity

Jérôme Weiss

Laboratoire de Glaciologie et Géophysique de l'Environnement, CNRS  
38402 St Martin d'Hères Cedex, France

As suggested by its very name and by smooth macroscopic stress-strain or creep curves, the classical view of plastic “flow” in crystalline materials is that of a smooth and homogeneous process. Yet, intermittency of plastic activity has been known for a long period of time. For example, it was described in Zn single crystals as early as 1932. However, these observations remained marginal, as the observed fluctuations were seen as sufficiently small and independent of one another to add at random to a smooth overall response. A fundamentally different picture emerged during the last few years, that of a scale-free intermittent plastic activity characterized by power law distributions of dislocation avalanche sizes, time correlations and aftershock triggering as well as fractal patterns and complex space-time coupling. First experimental evidences came from acoustic emission (AE) experiments on deformed ice single crystals that showed power law distributions of AE amplitude and energy, where the maximum AE amplitude  $A_0$  of an event is a proxy of the strain increment carried by the avalanche. These results were first presented to the dislocation community at *Dislocations2000*. Since then, they have been supported by different modelling approaches including 2D and 3D discrete dislocation dynamics, phase-field or continuum models. Independent experimental support was obtained from compression tests on Ni micron-size single crystals that showed staircase-like stress-strain curves with power law distribution of step size.

All of these findings argue for a renewed viewpoint on crystalline plasticity, reminiscent of the concept of crackling noise describing out-of-equilibrium physical systems with bursts of activity (avalanches), in close vicinity to criticality. Recent monitoring of the plastic deformation of metallic single crystals (Cu, Zn, Cd) from AE and micro-extensometry revealed the universal character for such intermittent plasticity: extreme fluctuations appear to be the rule, not the exception. We note however that (i) the existence of an internal length scale in polycrystals, the average grain size, limits the amplitude of fluctuations and therefore breaks down the scale invariance, and that (ii) there are still doubts on whether this critical dynamics develops in materials with low dislocation mobility (because of e.g. high lattice friction), when obstacles to dislocation motion (such as Peierls barriers, microparticles) either hinder or slow down free rearrangements of the dislocation population.

In this presentation, I will review the story of this “crackling plasticity” since *Dislocations2000*, and will discuss its consequences in terms of modelling of plastic deformation.

## Dislocation dynamics, mean free path and slip avalanches in fcc crystals

Benoit Devincré<sup>1</sup>, Ladislav P. Kubin<sup>1</sup> and Thierry Hoc<sup>2</sup>

<sup>1</sup> LEM, CNRS-ONERA, 29 Av. de la Division Leclerc, BP 72,  
92322 Châtillon Cedex, France

<sup>2</sup> Laboratoire MSSMat., Ecole Centrale Paris, Grande Voie des Vignes,  
92295 Châtenay-Malabry Cedex, France

At the micrometer scale, plastic deformation happens by intermittent bursts or slip avalanches, which are characterized by scale-free behavior within a bounded domain of amplitudes or energies. The probability density of slip avalanches, their processes of initiation and termination and their contribution to dislocation storage during plastic flow are investigated with dislocation dynamics (DD) simulations. For this purpose, a representative volume element of copper with periodic boundary conditions is strained along high symmetry orientations. The distribution of avalanches measured with DD simulations exhibits, for all the tested orientations, a scaling exponent of 1.6 similar to what is reported in the literature. However, the corresponding average amplitude is found to be orientation-dependent. Furthermore, for all tested orientations, the ratio of the dislocations mean free path, as defined in continuum plasticity models, to the average characteristic length traveled by dislocations during slip avalanches appears to be a constant. This constant ratio shows that an implicit coarse-graining procedure is performed when measuring dislocation mean free path in DD simulations or consistently that the discrete nature of plastic deformation in fcc crystals can be incorporated into continuum models.

# Statistical Characterization of Dislocation Systems with Dislocation Dynamics Simulation

Ferenc F. Csikor and István Groma  
Department of Materials Physics, Eötvös University Budapest  
Pázmány Péter sétány 1/a, H-1117 Budapest, Hungary

Thomas Hochrainer  
Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

Christian Motz  
Erich Schmid Institute of Materials Science, Austrian Academy of Sciences  
A-8700 Leoben, Austria

Daniel Weygand  
Institut für die Zuverlässigkeit von Bauteilen und Systemen, Universität Karlsruhe (TH)  
Kaiserstrasse 12, 76131 Karlsruhe, Germany

Michael Zaiser  
Centre for Materials Science and Engineering, The University of Edinburgh  
The King's Buildings, Sanderson Building, Edinburgh EH8 3JL, UK

Stefano Zapperi  
CNR-INFM, S3, Dipartimento di Fisica, Università di Modena e Reggio Emilia  
via Campi 213/A, I-41100, Modena, Italy

The usual goal of performing Discrete Dislocation Dynamics (DDD) simulations is to study the microscopic phenomenology of bulk or microcrystal deformation. Here we present another utilization of the DDD methodology, to provide input to statistical theories of crystal plasticity.

The last ten years saw the steady development of continuum bulk crystal plasticity theories based on the statistical mechanics of many-dislocation systems. One of the most important findings in strongly simplified two-dimensional slip geometries was the recognition that gradient terms, needed to describe size effects in continuum theories, are the direct consequences of short-range dislocation correlations. With the advent of three-dimensional generalizations of these continuum plasticity theories it became necessary to study the pair correlation functions of the complete three-dimensional dislocation problem. In this paper we present DDD simulation results for the range of dislocation pair correlations in fcc single crystals.

Recently, the intermittent plastic deformation of microcrystals has attracted a lot of interest. As typical for critical phenomena in general, many observed statistical characters of microcrystal plasticity show scale-free characteristics. Experimental results for the probability distribution of strain burst sizes also fall into this category, which would paradoxically indicate the largest strain bursts to be observable in macroscopic samples. With the DDD simulation of the quasi-static plastic deformation of a large number of fcc microcrystals we established the existence of an upper cut-off for the scale-free distribution of strain burst sizes. By varying the system size, the slip geometry, the temperature and the loading conditions, a universal functional form for the strain burst size distribution function was also demonstrated for a wide range of different conditions.

**Preference:** Oral presentation

**Presenter:** Ferenc F. Csikor

# Topology and transport in driven vortex lattices

Paolo Moretti and M. Carmen Miguel

*Departament de Física Fonamental, Facultat de Física, Universitat de Barcelona,  
Martí i Franquès 1, E-08028 Barcelona, Spain, email: paolo.moretti@ub.edu*

PACS numbers: 74.25.Qt, 61.72.Mm

Recent studies have established a tight connection between driven vortex lattices in Type II superconductors and plastically deforming crystals. Both the atomistic and the mesoscopic behavior of disordered vortex assemblies under the effect of applied external currents implies topological rearrangements which involve dislocations and dislocation assemblies and result in the emergence of polycrystalline and amorphous states.

In this work we would like to emphasize the close relation between topological adjustments of the vortex lattice and its electrodynamic response. We perform a numerical study of the critical current by tuning certain relevant parameters, namely the magnetic field, the density of defects and, most importantly, the typical disorder strength, or pinning force.

In the case of weak pinning interactions, the dynamics of dislocation assemblies is the relevant mechanism that accounts for the collective motion of the vortex array. Dislocations rearrange into grain boundaries, accounting for the emergence of polycrystalline order. We prove that grain boundary interactions with defects are responsible for a non-trivial dependence of critical currents on the average defect density and we are able to corroborate previous analytical results which predicted the observation of individual and collective pinning regimes. Dislocation motion is associated with non trivial  $1/f$ -noise features, which signal the emergence of correlated deformation patterns and strain avalanches.

In the case of higher defect strengths, instead, the vortex assembly loses lattice ordering and falls into a completely disordered phase. The consequent increase in the number of degrees of freedom results in a huge increase of the critical current. Depinning is now strongly heterogeneous, accompanied by a sharply discontinuous transition and jerky individual vortex dynamics. For applied currents right above the depinning threshold, the flowing state is anticipated by a moving state in which only a restricted number of vortices is in motion and plastic activity is strongly localized.

**Preference:** Oral presentation

**Presenter:** Paolo Moretti