

Technical Program

MMM 2008
*Fourth
International Conference*
MULTISCALE MATERIALS MODELING
OCTOBER 27-31, 2008 • TALLAHASSEE, FLORIDA, USA

Organised and Hosted by
The Department of Scientific Computing and
Florida State University

DEPARTMENT OF
Scientific
COMPUTING



Technical Program

Plenary Talks

Session M-A (Anter El-Azab, Chair)

Monday, 27 October 2008

9:00 a.m.

Meeting Room A-3

H. Kroto

Architecture in nanospace

Session M-E (Ladislav Kubin, Chair)

Monday, 27 October 2008

5:30 p.m.

Meeting Room A-3

S. Suresh

Nanomechanics and the study of human disease states

Session T-A (Ben Larson, Chair)

Tuesday, 28 October 2008

9:00 a.m.

Meeting Room A-3

N. Ghoniem

Multiscale Modeling of the Mechanical Behavior of Structural Materials in Nuclear Energy Systems

Session T-E (Nasr Ghoniem, Chair)

Tuesday, 28 October 2008

5:30 p.m.

Meeting Room A-3

B. Larson

Linking multiscale materials modeling with experiment at the mesoscale using 3D X-ray microscopy

Session W-A (Max Gunzburger, Chair)

Wednesday, 29 October 2008

9:00 a.m.

Meeting Room A-3

W. E

Some mathematical and numerical issues in multiscale modeling

Session W-E (Bill Curtin, Chair)

Wednesday, 29 October 2008

5:30 p.m.

Meeting Room A-3

P. Gumbsch

Making and breaking of chemical bonds under mechanical load

Session Th-A (Michael Zaiser, Chair)

Thursday, 30 October 2008

9:00 a.m.

Meeting Room A-3

S. Roux

Depinning Transition in Solid Mechanics

Session Th-E (Peter Gumbsch, Chair)

Thursday, 30 October 2008

5:30 p.m.

Meeting Room A-3

T. Belytschko

Multiscale computations of fracture: quantum to continuum

Session F-A (Steve Zinkle, Chair)

Friday, 31 October 2008

8:20 a.m.

Meeting Room A-3

D. Bacon

In pursuit of imperfection: can modelling help?

Session F-B (Erik van der Giessen, Chair)

Friday, 31 October 2008

9:20 a.m.

Meeting Room A-3

J. Fish

Coupling of Atomistic and Continuum Scales

Symposium 1
Mathematical issues in multiscale materials modeling

Session M-B (Max Gunzburger, Chair)

Monday, 27 October 2008

Meeting Room B

R. Caflisch
Multiscale Methods for Fluid and Plasma Dynamics
10:20 a.m.

J. W. Barrett, D. Knezevic, E. Süli
Kinetic Models for Dilute Polymers: Analysis, Approximation and Computation
10:50 a.m.

P. Plechac
Coarse-graining of Macro-molecular Systems: Mathematical and Numerical Methods
11:20 a.m.

~~J. H. Maddocks, R. Manning,
L. Cotta Ramusino~~
A Path integral Formulation of DNA Looping Probabilities
11:50 a.m.

Session M-C (Mitch Luskin, Chair)

Monday, 27 October 2008

Meeting Room B

G. Friesecke, O. Junge
Mean Field Approximation of Transfer Operators in High-dimensional Conformation Dynamics
1:40 p.m.

X. Blanc, C. Le Bris, P.-L. Lions
Some Recent Progress in Elliptic Homogenization
2:10 p.m.

Q. Du
Micro-macro FENE Models for Polymeric Materials and their Closure Approximations
2:40 p.m.

L. Berlyand
Homogenization with Nonseparated Scales
3:00 p.m.

Session M-D (Weinan E, Chair)

Monday, 27 October 2008

Meeting Room B

I. Dabo, E. Cancès, Y. Li, N. Marzari
Toward Multiscale Modelling and Simulation of Fuel Cells
3:40 p.m.

C. J. Garcia-Cervera, J. Lu, W. E
Sub-linear Scaling Algorithms for the Study of the Electronic Structure of Materials
4:10 p.m.

M. Griebel, J. Hamaekers, F. Heber
BOSSANOVA: A bond order dissection approach for efficient electronic structure calculations
4:40 p.m.

Session T-B (Rich Lehoucq, Chair)

Tuesday, 28 October 2008

Meeting Room B

J. T. Oden, S. Prudhomme,
P. T. Bauman, L. Chamoin
Adaptive Control of Modeling Error for Multiscale Simulations
10:20 a.m.

A. El-Azab
A New Frontier of Kinetic
Theory Applications in Solid
Mechanics—The Discrete-Continuum
Connection in Dislocation Dynamics
10:50 a.m.

V. Gavini
Electronic Structure Calculations at
Macroscopic Scales
11:20 a.m.

D. Aubry, A.-L. Hamon
A Numerical Bridge Between Quantum
and Molecular Dynamics based on the
Ehrenfest Dynamics
11:40 a.m.

L. Chamoin, S. Prudhomme, J. T. Oden,
P. T. Bauman
On a Stochastic Approach for Atomic-
to-Continuum Coupling Methods
12:00 p.m.

Session T-C (Weinan E, Chair)
Tuesday, 28 October 2008
Meeting Room B

M. Luskin, M. Arndt, M. Dobson
Mathematical Validation and Algorithms
for the Quasicontinuum Method
1:40 p.m.

R. E. Miller, E. B. Tadmor, M. Luskin
Comparing the Accuracy and Efficiency
of Multiscale Methods
2:10 p.m.

J. P. Reese, M. Gunzburger
1D Atomistic-to-Continuum Coupling
via Optimization
2:40 p.m.

Y. Zhang, M. Gunzburger
Approximating the quasicontinuum
method using quadrature rules
3:00 p.m.

Session W-B (Mitch Luskin, Chair)
Wednesday, 29 October 2008
Meeting Room B

P. Ming
Analysis of Quasicontinuum Method
10:20 a.m.

K. Fackeldey, D. Krause, R. Krause
Quadrature and Implementation of the
Weak Coupling Method
11:00 a.m.

R. Lehoucq, S. Silling
Peridynamics, Molecular Dynamics,
and Classical (nonlinear) Elasticity
11:20 a.m.

M. L. Parks, P. Seleson
Molecular dynamics at Larger Scales:
Peridynamics as an upscaling of
molecular dynamics
11:50 a.m.

X. Blanc, C. Le Bris, F. Legoll, C. Patz
Coarse-graining the Free energy of
Atomistic Systems: a simple case
12:20 p.m.

Session Th-B (Max Gunzburger, Chair)
Thursday, 30 October 2008
Meeting Room D

H. Garmestani
Inverse Microstructure Design Based on
Statistical correlation functions
10:20 a.m.

Y. Wang,, V. Lasrado, D. Alhat
A Review of Recent Transition State
Search Methods in Phase Transition
Simulation
11:00 a.m.

~~V. Melicher, J. Busa~~
~~Finite Element Heterogeneous~~
~~Multiscale Method and Micromagnetism~~
11:20 a.m.

R.C. Picu, M.A. Soare
Homogenization of Stochastic Fractal
Microstructures
11:40 a.m.

Poster Session W-D (Anter El-Azab,
Chair)
Wednesday, 29 October 2008
3:20-5:20 p.m.
Arena Access Area

X. Chen, M. Gunzburger
Finite Element Methods for a
Peridynamic Model of Mechanics
Poster

P. Seleson, M. Gunzburger
Bridging Methods and Boundary
Treatment for AtC Coupling Problems
Poster

Abdmanam Elmaryami
Effect of Thermal Cycling on Hardness
of Plain Carbon Steel
Poster

O. U. Okeke
Electronic Structure calculations of
Novel Spinel Oxynitrides
Poster

L. Liu
The Attainability of
Hashin-Shtrikman Bounds
Poster

N. Castin, L. Malerba
New Approach To Model Point Defects
Migration Using A Monte-Carlo
Paradigm Coupled With Artificial
Intelligence
Poster

Z. Dudas
Regression Possibilities of Isothermal
Transformation (IT) and Continuous
Cooling (CC) Transformation Diagrams
using T-t Elements
Poster

S. Fitzgerald, D. Nguyen-Manh,
Z. Dudas
Analytic Solution of the Discrete Double
Sine-Gordon Model: application to
crowdion migration in the bcc
transition metals
Poster

A. V. Barashev, S. I. Golubov,
D. J. Bacon, Y. N. Osetsky, R. E. Stoller
Generalisation of the Diffusion-Reaction
Theory for Inclusion Of Complexes with
Long-Range Interaction Range
Poster

Symposium 2
Statistical methods for material deformation and failure

Session W-B (M.C. Miguel, Chair)
Wednesday, 29 October 2008
Meeting Room C

T.C. Lubensky
Theory of Nematic and Smectic Elastomers
10:20 a.m.

A.H.W. Ngan
Athermal Statistical Mechanics for Material Elastostatics and Deformation
10:50 a.m.

R. Gröger, T. Lookman, A. Saxena
Mesoscopic description of martensitic phase transformations mediated by dislocations using the Landau-Ginzburg theory
11:20 a.m.

L. Laurson, M.-C. Miguel, M. J. Alava
Heterogeneous Dynamics Near Dislocation Jamming
11:40 a.m.

P. Moretti, M. C. Miguel
Topology and Transport in Driven Vortex Lattices
12:00 p.m.

A. M. Mughal, M. A. Moore
Topological Defects in the Crystalline State of One-component Plasmas of Non-uniform Density
12:20 p.m.

Session W-C (M. Alava, Chair)
Wednesday, 29 October 2008
Meeting Room C

J. P. Sethna, S. Limkumnerd
Walls formed by Bending: Grain Boundaries and Cell Walls from Continuum Plasticity
1:40 p.m.

T. Hochrainer, P. Gumbsch, M. Zaiser
A Non-Linear Multiple Slip Theory in Continuum Dislocation Dynamics
2:00 p.m.

J. Deng, A. El-Azab
Theoretical and Computational Modeling of the Statistics of Internal Elastic Fields in 3D Dislocation Systems
2:20 p.m.

F. F. Csikor, I. Groma, T. Hochrainer, D. Weygand, M. Zaiser
3D Dislocation Pair Correlation Functions from DDD Simulations
2:40 p.m.

Session Th-B (I. Groma, Chair)
Thursday, 30 October 2008
Meeting Room B

D. Bonamy, S. Santucci, L. Ponson, K.-J. Maloy
Intermittent Crack Growth in Heterogeneous Brittle Materials
10:20 a.m.

P. K. Nukala, S. Zapperi, M. J. Alava, S. Simunovic
Analysis of Fracture Roughness using 2D Beam Lattice Systems
10:50 a.m.

M. Zaiser, P. Moretti, A. Konstantinidis,
E.C. Aifantis
Shear failure of thin films on disordered
substrates: Nucleation and propagation
of interfacial shear cracks
11:20 a.m.

M. Alava, P. K. Nukala, S. Zapperi
Strength of Heterogeneous Materials
with Flaws
12:00 p.m.

Session Th-C (T. Lubensky, Chair)
Thursday, 30 October 2008
Meeting Room B

C. E. Maloney, K. M. Salerno,
M. O. Robbins
Deformation in disordered solids:
Correlations in displacement derivatives
and avalanche distributions
1:40 p.m.

P. Schall
Colloidal Glasses Visualize Multiscale
Plasticity in Amorphous Solids
2:10 p.m.

C. E. Maloney
Defects in Amorphous Solids
2:40 p.m.

J. Kumar, M. Ciccotti,
G. Ananthakrishna
Dynamics of Cracking Noise during
Peeling of an Adhesive Tape
3:00 p.m.

Session Th-D (M. Robbins, Chair)
Thursday, 30 October 2008
Meeting Room B

M. Itakura, H. Kaburaki, M. Yamaguchi,
T. Kadoyoshi
Coupled Simulation of Grain Boundary
Decohesion and Hydrogen Segregation

3:40 p.m.

S. Zapperi, M. Alava, P. Nukala
Statistical Models for Planar Crack
Propagation
4:00 p.m.

D. Gómez-García, E. Zapata-Solvas,
A. Domínguez-Rodríguez
A Statistical Approach to High-
Temperature Plasticity of Ceramic
Polycrystals
4:20 p.m.

I. Corominas, L. Laurson, M. Alava,
M. C. Miguel
Statistical Behavior of Internal Stress in
2D Dislocation Assemblies
4:40 p.m.

Poster Session W-D (M.C. Miguel and I.
Groma, Chairs)
Wednesday, 29 October 2008
3:20-5:20 p.m.
Arena Access Area

X. Li
Effect of Stacking Fault Energy on
Defect of Accumulation in
Stainless Steels
Poster

R.C. Picu, H. Hatami-Marbini
Scaling of the Non-Affine Deformation
of Random Fiber Networks
Poster

Y. Chen, W. S. Choi, S. Papanikolaou,
S. Limkumnerd, J. P. Sethna
Predictions of a continuum dislocation
density theory: cell wall and grain
boundary evolution in crystals
Poster

~~D. Tonks, J. Bingert, V. Livescu~~

~~Roughness of Damage Paths and
Cavities in Shock Loaded Tantalum~~
Poster

J. Chevy, P. Duval, M. Fivel,
J. Weiss, P. Bastie
Heterogeneities Induced by Dislocation
Multiplication in Ice: Experimental and
Numerical Evidences
Poster

Symposium 3 **Multiscale mechanics**

Session M-B (Bo Yang, Chair)

Monday, 27 October 2008

Meeting Room A3

M. Cho, S. Yang, J. Choi
Development of sequential multi-scale
analysis for nano structured materials
10:20 a.m.

Y. Nakasone
Polycrystal Plasticity Analysis of
Bimodal Structures Considering the
Three-Stage Characteristics of the
Resolved Shear Stress vs. Strain Curves
of Individual Grains
11:00 a.m.

M. Arroyo, I. Arias
Mesoscopic modelling and size effect
for the mechanics of multi-walled carbon
nanotubes
11:20 a.m.

A. Montazeri, R. Naghdabadi
Investigation the stability of SWCNT-
polymer composites in the presence of
CNT geometrical defects using
multiscale modeling
11:40 a.m.

T. Vaughan, C. McCarthy
Development of Statistically Equivalent
Representative Volume Elements for
Multi-scale Modeling of Composite
Materials
12:00 noon

Session M-C (Ron Peerlings, Chair)

Monday, 27 October 2008

Meeting Room A3

S. Ricker, J. Mergheim, P. Steinmann

On the Multi-Scale Computation of
Defect Driving Force
1:40 p.m.

K. Terada, I. Watanabe
Numerical Material Testing for Strength
Evaluation of Polycrystalline Metals
2:10 p.m.

A. Gaubert, S. Forest
Modeling size effect dependence on
mechanical behaviour using a Cosserat
crystal plasticity framework
2:40 p.m.

N. Nicaise, S. Berbenni, F. Wagner,
M. Berveiller, X. Lemoine
Combined Effects of Crystallographic
and Grain Size Heterogeneities on
Plasticity of Polycrystalline IF Steels
3 :00 p.m.

Session M-D (Vasily Bulatov, Chair)
Monday, 27 October 2008
Meeting Room A3

G. Ziegenhain, A. Hartmaier,
H. M. Urbassek
Onset of Plasticity Under
Nanoindentation: Influence of the
Interatomic Potential
3:40 p.m.

Y. Umeno
Effect of Surface Structure on Strength
of Si Thin Film
4:00 p.m.

B. Yang
Dislocation-guided Dynamics of Surface
Defects on a Multilayered Si-Ge
Heterostructure
4:20 p.m.

Session T-B (T. Arsenlis, Chair)
Tuesday, 28 October 2008

Meeting Room A3

V. V. Bulatov
Dislocation Dynamics for Engineering
Applications
10 :20 a.m.

M.P. Ariza, M. Ortiz
Dilute Discrete Dislocation Dynamics
10:50 a.m.

C. Motz, D. Weygand, P. Gumbsch
Size and Bauschinger Effects in Micro-
bending: A 3D Discrete Dislocation
Dynamics Study
11:20 a.m.

J. Segurado, J. Llorca, I. Romero
An analysis of the size effect in void
growth in single crystals using discrete
dislocation dynamics
11:40 a.m.

R.H.J. Peerlings, Y. Kasyanyuk, A. Roy,
M.G.D. Geers
Mesoscale Modelling of Dislocation
Pile-up Based on Discrete Interactions
12:00 p.m.

Session T-C (Peter Chung, Chair)
Tuesday, 28 October 2008
Meeting Room A3

G. Lasko, Y. Y. Deryugin, S. Schmauder
The role of the edge effects in the strain
localization evolution in polycrystals on
the mesolevel
1:40 p.m.

R. Elliott, N. Triantafyllidis, J. Shaw
An Effective Interaction Potential Model
of Stress- and Temperature-induced
Martensitic Transformations in
Perfect Bi-atomic Crystals
2:00 p.m.

R. Brenner, R. A. Lebensohn,
O. Castelnau
Influence of the elastic anisotropy on the
initial yielding of polycrystals
2:20 p.m.

N. Bonfoh, P. Lipinski
Micromechanical Modeling of Materials
containing Intra-crystalline Particles
2:40 p.m.

R. A. Lebensohn, C. N. Tomé, C. S.
Hartley, O. Castelnau, S. A. Maloy
Selfconsistent Modelling of the
Mechanical Response of Viscoplastic
Polycrystals Deforming by Glide and
Climb
3:00 p.m.

Session W-B (Bill Curtin, Chair)
Wednesday, 29 October 2008
Meeting Room A3

R. Kobayashi, T. Nakamura, S. Ogata
Large-Scale Simulation of Oscillating
Metal-Nanorod: Application of the
Hybrid Molecular-Dynamics/Coarse-
Grained-Particle Approach
10:20 a.m.

Y. Chen, L. Xiong
Reformulation of Continuum Mechanics
to Include Multiple Length/Time Scales
10:40 a.m.

~~C. Arévalo, Y. Kulkarni, M.P. Ariza,
M. Ortiz, J. Knap, J. Marian~~
Hot Quasicontinuum calculations of
nanovoids evolution under volumetric
expansion
11:00 a.m.

D. Nicholson, S. Namilaie,
P. K.V.V. Nukala, Y.N.Osteskiy,
C.Y.Gao, D.J. Keffer

Coupling Atomistic and Continuum
Descriptions: Continuity of Energy Flux
and Correlation
11:20 a.m.

K. Jolley, S. P.A. Gill
Atomistic/continuum models for
multiscale heat conduction
11:40 a.m.

P. W. Chung, M. F. Macri
A Comparative Study of Multiscale
Modeling of Generalized Finite
Elements and Molecular Dynamics
12:00 p.m.

M. Anitescu, A. El-Azab, P. Zapol,
D. Negrut
Reduced Models Obtained by Nonlocal
Quasi-continuum-like Approaches
12:20 p.m.

Session W-C (Tom Arsenlis, Chair)
Wednesday, 29 October 2008
Meeting Room A3

J. Morris, K. Magid, N. Tamura,
J. Florando, D. Lassila, M. leBlanc
Mapping Mesoscale Heterogeneity in the
Deformation of Single Crystal Copper
1:40 p.m.

S. Puri, A. Acharya
Continuum Modeling of Plastic
Deformation in Polycrystalline Thin
Films
2:10 p.m.

C. Perrin, T. Richeton, S. Berbenni,
M. Berveiller, H. Vehoff
Role of Intra-granular Plastic Slip
Heterogeneities on Lattice Rotations:
comparisons between experimental
measurements and a new
micromechanical modeling
2:40 p.m.

N. Cordero, E. Busso, S. Forest
Higher Order Conditions at Grain
Boundaries: Finite Element Simulations
of Polycrystal Behavior
3:00 p.m.

Session Th-B (Nathan Barton, Chair)
Thursday, 30 October 2008
Meeting Room A3

T.W. Wright, K.T. Ramesh
Microstructural Aspects of Ductile
Rupture in Solids
10:20 a.m.

J. Hua, A. Hartmaier, M. Duchaineau
Determination of Burgers Vectors from
Atomistic Data
10:40 a.m.

G. Moras, L. C. Ciacchi, C. Elsässer,
A. De Vita
Modelling the Growth of Hydrogen-
Induced Platelets in Silicon with the
“Learn On The Fly” Multiscale
Molecular Dynamics Technique
11:00 a.m.

O. R. de la Fuente
Heterogeneous Dislocation Nucleation
in Defective Metal Surfaces During
Nanoindentation
11:20 a.m.

T. Hirouchi, T. Takaki, Y. Tomita
New Computational Technique for
Evaluating Deformation of
Nanocrystalline Metal using Phase Field
Crystal Method
11:40 a.m.

J. Ghanbari, R. Naghdabadi
Modeling the interphase layer between
CNT and matrix in Nanocomposites
using nonlinear large deformation
hierarchical multiscale

12:00 p.m.

Session Th-C (T. Arsenlis, Chair)
Thursday, 30 October 2008
Meeting Room A3

A. Widjaja, A. Needleman,
E. Van der Giessen
Grain Size Effects in the Wedge
Indentation of Polycrystals: a Discrete
Dislocation Analysis
1:40 p.m.

W. Curtin
Multi-scale plasticity modeling: from
atoms to continuum crystal plasticity
2:10 p.m.

N. R. Barton, J. V. Bernier, J. Knap
Applications of Adaptive Sampling in
Multi-scale Simulations
2:40 p.m.

A. Ramasubramaniam, M. Itakura,
M. Ortiz, E. A. Carter
Modeling Hydrogen Embrittlement in
Metals: Coupling Quantum Mechanical,
Empirical Potential and Kinetic Monte
Carlo Approaches
3:00 p.m.

Session Th-D (Don Nicholson, Chair)
Thursday, 30 October 2008
Meeting Room A3

M. Chabaat, H. Hamli Ben Zahar
Stress analysis during the interaction
between dislocations and a main crack:
Case of a bi-material
3:40 p.m.

K. E. Aifantis, A. A. Konstantinidis,
M. Zaiser
Damage Evolution in Foams
4:00 p.m.

S. Ogata, Y. Abe, R. Kobayashi
Adaptive Embedding of the Electronic-
Density-Functional-Theory in the
Classical Molecular Dynamics:
Application to Nano-Indentation
4:20 p.m.

I. Tirtom, T. Shoji
Python Based Combined Continuum-
atomic Modeling for Single Crystal
Nickel
4:40 p.m.

Poster Session T-D (Peter Chung and T.
Arsenlis, Chairs)

*Tuesday, 28 October 2008
3:20-5:20 p.m.
Arena Access Area*

M. K. Saraswat
Investigating the Time Dependency of
the Viscoelastic Bulk Modulus using
Gnomix PVT Apparatus
Poster

H. Tanaka, Y. Shibutani
Size Effect of Finite Deformable
Nanopillar by Focused-ion-beam
Chemical Vapor Deposition
Poster

S. Hara, T. Take, S. Izumi, S. Sakai
Reaction Pathway Analysis of
Dislocation-Interface Interactions in
Cu-Ni Multilayered Systems
Poster

O. Castelnau, P. Duval, M. Montagnat,
R. Brenner
Elasto-Viscoplastic Micromechanical
Modelling of the Transient Creep of Ice

Poster

X. Xie., H. Zhou., J. Zhu, J. Guo, S. Yan
Synthesis for Ceramic Oxides
Poster

A. Agrawal, R. Saha
Evaluation of influence of size of
inclusion on the Effective Material
Property of Particle reinforced
Composites
Poster

Q. H. Bui, S. Ramtani, G. F. Dirras
Generalized self consistent
polycrystalline model applied to
Heterogeneous materials exhibiting log
normal grain size distribution
Poster

J. Vorel, M. Sejnoha
Two Step Homogenization of Thermal
Conductivities for Macroscopically
Orthotropic C/C Composites
Poster

M. O. Steinhauser
Failure of Granular Materials under
Impact – Multiscale Simulations and
High-Speed Experiments
Poster

M. Černý, J. Pokluda, J. Horníková,
P. Šandera
Multiscale Model of Nanoindentation
Test in Cu and Ni
Poster

D. Terentyev, D.J. Bacon,
P. Grammatikopoulos, Y.N. Osetsky
Hardening by completely and partially
absorbed $\frac{1}{2}\langle 111 \rangle$ and $\langle 100 \rangle$ dislocation
loops reacting with dislocations in α -Fe
Poster

G. Bonny, D. Terentyev, L. Malerba
 α - α' phase separation in Fe-Cr alloys and
its impact on mechanical properties: An
atomistic study
Poster

E. Clouet, L. Ventelon, F. Willaime
Dislocation Core Fields and Elasticity
Theory: The Screw Dislocation in Iron
Poster

X. Yuan
On micromechanical models of
nonlocal media
Poster

Y.-G. Cho, J.-Y. Kim, P.-R. Cha,
J. K. Lee, H. N. Han
Analysis of Transformation Plasticity
Using a Finite Element Model Coupled
with a Phase Field Method
Poster

C. Gan, S.-S. Quek
Al atomistic dislocation simulations
using a tight-binding method
Poster

S. Knell, M. Sauer, K. Thoma
Numerical Analysis of Ceramics under
Impulsive Loads at Grain Scale
Poster

A. Butz, T. Rist, B. Springub, F. Roters,
S. Schultz
Virtual Processing of Dual Phase Steels
– A Microstructure Based Simulation
Approach
Poster

R. Regueiro
On a Finite Strain Micromorphic
Plasticity Model for Bound Particulate
Materials
Poster

M. Verdier
Microyield Behaviour of Metallic
Multilayers
Poster

P. Mueller, P. Spätig
Numerical investigations of compact
tension fracture specimens
Poster

T. Antretter, W. Pranger, T. Waitz,
F.D. Fischer
An Energy Approach to Determine the
Martensite Morphology in Nano-
Structured NiTi Alloys
Poster

M. A. S. Qidwai, A. C. Lewis,
A. B. Geltmacher
Towards identification of
microstructure-property correlations
in a titanium alloy using image-based
modeling
Poster

D. P. Do, N. Belayachi, D. Hoxha,
A. Giraud
Numerical and analytical
homogenisation approach for modeling
mechanical behaviour of heterogeneous
geomaterials
Poster

M. Davies, A. Lew
An Adaptive Coarse-Graining Scheme
for the Simulation of Elastomer
Networks
Poster

T. Arsenlis, V. Bulatov, G. Hommes,
M. Rhee, M. Tang
Dislocation Quasi-Statics: Implicit Time
Integration for Dislocation Dynamics
Simulations
Poster

P. R. Barry, P. Y. Chiu, S. S. Perry,
W. G. Sawyer, S. R. Phillpot,
S. B. Sinnott
Orientation Dependence of Friction
in PTFE
Poster

J. Fan, M. Chinappi
Multiscale Analysis of Cell-Gold
Adhesion
Poster

J. Tan, C. Li, C. Sun, S. Ying
Stress relaxation and dynamic strain
aging of Zr-Sn-Nb alloy
Poster

J. Rahmoun, J. Halgrin, F. Chaari,
E. Markiewicz, P. Drazetic
Micromechanical modeling of the
anisotropy of elastic biological
composites - Theory and fundamental
concepts
Poster

T. Liang, W. G. Sawyer, S. S. Perry,
S. R. Phillpot, S. B. Sinnott
Atomistic Simulations of Tribology at
Sliding MoS Surfaces
Poster

J. A. Alvarado-Contreras, M. A. Polak,
A. Penlidis
Modelling Damage of the Crystalline
Phase in Semicrystalline Polyethylene
Poster

K. Cook-Chennault
Composite piezoelectric structures used
for energy harvesting
Poster

X. Zeng, A. Hartmaier
Modeling the Competition between
Inter- and Intra-granular Fracture in

Tungsten Polycrystals at Ambient
Temperature
Poster

~~M. Jerabek, Z. Major~~
~~On the micromechanical deformation of~~
~~particle filled polypropylene compounds~~
Poster

Symposium 4
Multiscale modeling of microstructure evolution in materials

Session M-B (Somnath Ghosh, Chair)

Monday, 27 October 2008

Meeting Room A2

B. Devincre, L. P. Kubin, T. Hoc
Dislocation Mean Free Paths and Storage During Plastic Flow: A Study by Dislocation Dynamics Simulations
10:20 a.m.

D. M. Dimiduk, C. Woodward, S. I. Rao, M. D. Uchic, T. A. Parthasarathy, R. LeSar, E. Nadgorny
Stochastic Flow and Size Effects in Microcrystal Plasticity
10:50 a.m.

D. Mordehai, E. Clouet, M. Fivel, M. Verdier
Introducing Dislocation Climb by Bulk Diffusion in Discrete Dislocation Dynamics Simulations
11:20 a.m.

S. S. Quek, Y.-W. Zhang, Y. Xiang, D. J. Srolovitz
Dislocations evolution in hetero-epitaxial multilayers
11:40 a.m.

D. Weygand, J. Senger, P. Gumbsch, O. Kraft
Plasticity Of Micro-samples: Discrete Dislocation Dynamics Study On The Size Effect Under Uniaxial Loading Conditions
12:00 p.m.

Session M-C (Dennis Dimiduk, Chair)

Monday, 27 October 2008

Meeting Room A2

P. Dawson
Modeling the Evolution of Intragrain Lattice Orientation Gradients and Yield Asymmetries in Polycrystalline Solids
1:40 p.m.

S. Ghosh, D. S. Joseph, P. Chakraborty
Crystal Plasticity Models with Multi-Time Scaling for Cyclic Deformation of Polycrystalline Metals
2:10 p.m.

C. Schäfer, V. Mohles, G. Gottstein
Through-Process Texture and Microstructure Modeling of AA3103 from Hot Rolling to Final Annealing
2:40 p.m.

A. Prakash, R. Lebensohn
Comparison of two full field approaches for modeling of Microstructure evolution of polycrystals
3:00 p.m.

Session M-D (Benoit Devincre, Chair)

Monday, 27 October 2008

Meeting Room A2

D. Jeulin
Morphological models of evolving microstructures
3:40 p.m.

V. I. Yamakov, E. Saether, E. H. Glaessgen
Multiscale Modeling of Fracture in Aluminum: Constitutive Relation for Interface Debonding from Atomistic Simulations
4:10 p.m.

B. Bakó, D. Weygand, M. Samaras,
W. Hoffelner, M. Zaiser
Dislocation depinning transition in a
dispersion strengthened steel
4:40 p.m.

Session T-B (Simon Philpot, Chair)
Tuesday, 28 October 2008
Meeting Room A2

S. M. Foiles, D. L. Olmsted, E. A. Holm
Using Atomistic Simulations To Inform
Mesoscale Simulations Of
Microstructural Evolution
10 :20 a.m.

E. Martinez
Synchronous Parallel Kinetic Monte
Carlo
11 :00 a.m.

T. G. Desai, B. Uberuaga, P. C. Millett,
D. Wolf
Stress-induced Phase Transformation in
Nanocrystalline UO₂
11:20 a.m.

M. Kabir, T. T. Lau, S. Yip,
K. J. Van Vliet
Kinetic Consequences of Point Defect
Energetics and Deformation
Mechanisms in Metastable Alloys
11:40 a.m.

H. M. Urbassek, L. A. Sandoval
Thermal and Elastic Properties of Fe
Nanowires
12:00 p.m.

Session T-C (Chris Woodward, Chair)
Tuesday, 28 October 2008
Meeting Room A2

G. Yingjun, H. Chuanggao, Z. Hailin,
W. Chunli, J. Xing

Atomic Bonding and Properties of
Metastable Phase in Al-Cu Alloy
1:40 p.m.

G. Bonny, P. Erhart, A. Caro,
R. C. Pasianot, L. Malerba,
M. Serrano de Caro
The impact of short range order on Fe-
Cr thermodynamics
2:00 p.m.

P. Olsson, C. Domain
Ab initio study of solutes and defects
in FeCr
2:20 p.m.

~~K. Scheerschmidt~~
~~Structural Reordering at Wafer Bonded~~
~~Interfaces and Quantum Dots using~~
~~Molecular Dynamics Relaxation with~~
~~Analytic Bond Order Potentials~~
2:40 p.m.

E. Saether, V. Yamakov, E. Glaessgen
An Embedded Statistical Method for
Coupling Molecular Dynamics And
Finite Element Analyses
3:00 p.m.

Session W-B (Tony Rollett, Chair)
Wednesday, 29 October 2008
Meeting Room A2

T. Bieler, M. Crimp, C. Boehlert,
L. Wang, Y. Yiyi, P. Eisenlohr,
F. Roters, D. Raabe, W. Liu, G. Ice,
D. Mason
Computational Modeling of Interactions
between Slip-systems and Grain
Boundaries that lead to Fracture
Initiation
10:40 a.m.

E.k M. Lauridsen, W. Ludwig,
R. W. Fonda, P. W. Voorhees

Experimental Observations of Evolving
Microstructures
11:00 a.m.

J. Wohlwend, C. Boswell, R. Behera,
S.R. Phillpot, S.B. Sinnott
Morphology and Growth Modes of
Metal-Oxides Deposited on SrTiO₃
11:30 a.m.

~~A. Diógenes, A. Corrêa, L. dos Santos,
V. Fernandes, C. Appoloni,
C. Fernandes
Porous Media Microstructure
Reconstruction using Pixel-based and
Objectbased Simulated Annealing –
Comparison with other Reconstruction
Methods
12 :00 p.m.~~

L. Yue, D. Weygand, P. Gumbsch
Grain Growth Modeling By A Three
Dimensional Vertex Dynamics
Simulation
12 :20 p.m.

Session W-C (Corbett Battaile, Chair)
Wednesday, 29 October 2008
Meeting Room A2

L. Saintoyant, L. Legras, Y. Bréchet
A Coupled Model for Recrystallisation
and Creep of Zirconium Alloys
1:40 p.m.

A. Rollett, S. Wilson, C. Roberts,
M. Upmanyu
Multiscale Modeling of Grain Growth
2:00 p.m.

B.-J. Lee, J.-W. Jang
Implementation of Grain Boundary
Property Database for Simulation of
Microstructure Evolution based on
Realistic Grain Orientations
2:20 p.m.

M. Kühn, M. O. Steinhauser
Modeling and Simulating Polycrystalline
Micro Structures: Power Diagrams vs.
Particles
2:40 p.m.

D. Weygand, M. Verdier, J. Lépinoux
Grain Growth Mechanisms in Bounded
Geometries
3:00 p.m.

Session Th-B (A. Finel, Chair)
Thursday, 30 October 2008
Meeting Room A2

D. Fuloria, P. D. Lee, W. Poole
Coupling of Direct Finite Element
Simulations of Semi-solid Behaviour
into Large Strain Deformation Processes
10:20 a.m.

C. C. Battaile, S. V. Prasad,
J. R. Michael
Self-Lubrication of Metal Surfaces by
Subgrain Evolution During Wear
10:40 a.m.

R. E. Logé, M. Bernacki, H. Resk,
Y. Chastel, T. Coupez
A Level Set Framework for the
Numerical Modelling of Primary
Recrystallization
11:00 a.m.

J. Belak, P.E.A. Turchi, M.R. Dorr,
D.F. Richards, J.-L. Fattebert,
M.E. Wickett, F.H. Streitz
Coupling of Atomistic and Meso-scale
Phase-field Modeling of Rapid
Solidification
11:20 a.m.

P.W. Voorhees, K-A Wu, K Thornton,
K.R. Elder

A Phase Field Crystal Model for Interfacial Evolution Under Stress
11:50 a.m.

Session Th-C (Dieter Wolf, Chair)
Thursday, 30 October 2008
Meeting Room A2

A. Finel, U. Salman, O. Shchyglo
A Phase Field Investigation of the Dynamics of the Martensitic Transition
1:40 p.m.

S. K. Rokkam, P. C. Millett,
D. W. Wolf, A. El-Azab
Phase Field Simulation of Void Growth in Irradiated Materials
2:20 p.m.

R. R. Mohanty, Y. Sohn
Phase Field Modeling of Interdiffusion Induced Microstructure Evolution Under Different Driving Forces
2:40 p.m.

K. G. Wang
Unified Modeling for Microstructure Evolution
3:00 p.m.

Session Th-D (Ke-gang Wang, Chair)
Thursday, 30 October 2008
Meeting Room A2

A. Viardin, B. Appolaire,
E. Aeby-Gautier, M. Gouné
Phase field modeling of martensite banding in dual phase steels
3:40 p.m.

R. Hariharaputran, D. T. Wu
Atomistic Simulation of Nucleation for Multiscale Modeling of Solidification
4:00 p.m.

P. C. Millett, T. Desai, D. Wolf,

S. Rokkam, A. El-Azab
Phase-Field Simulation of Microstructure and Void Evolution in Irradiated Materials
4:20 p.m.

V. Racherla, P. P. Castañeda
Multi-scale Modeling of Unoriented Thermoplastic Elastomers with Lamellar Morphology
4:40 p.m.

Poster Session T-D (J. Simmons, D. Weygand, Chairs)
Tuesday, 28 October 2008
3:20-5:20 p.m.
Arena Access Area

V. Taupin, S. Varadhan, C. Fressemegeas,
A. J. Beaudoin
Polarized Dislocation Structures and Directionality of Yield Point in Strain-aged Steels
Poster

M. Timonova, B. Thijssse
Modeling Silicon in Demanding Conditions by a New MEAM Potential
Poster

A. Yamanaka, T. Yamamoto, T. Takaki,
Y. Tomita
Multi-Phase-Field Study for Pearlite Transformation with Grain Boundary Diffusion
Poster

J. Mach, A. J. Beaudoin, A. Acharya
Texture Evolution & (Partial) Continuity of the Plastic Strain Rate
Poster

R. Elliott, S. Sorkin, E. Tadmor
A Quasicontinuum for Multilattice Crystals Exhibiting Martensitic Phase

Transformations: Cascading Cauchy-
Born Kinematics
Poster

B. I. Jung
Finite Element Method and
Experimental Approaches in Drawing of
Hypereutectoid Steel
Poster

J. Marian, J. Knap
Breakdown of Self-Similar Hardening
Behavior in Au Nanopillar
Microplasticity
Poster

M. Emelianenko, D. Golovaty,
D. Kinderlehrer
Texture Evolution: New Perspectives
Poster
A. M. Dongare, L. V. Zhigilei
Kinetic Monte Carlo Simulation Study
of The Evolution of Surface Structures
During Sub-monolayer Thin Film
Growth of Ge on Clean and Patterned
Si(001) Substrates
Poster

M. I. Pascuet, J. R. Fernández,
A. M. Monti
Many Body Atomic Interaction for
Uranium
Poster

A. Kuksin, G. Norman, V. Pisarev ,
V. Stegailov, A. Yanilkin
Molecular Dynamics Simulations and
Kinetic Models of Fracture under High
Strain Rate
Poster

A. Y. Kuksin, G. E. Norman,
V. V. Stegailov, A. V. Yanilkin
The Influence of Temperature on
Plasticity of Al Alloys: Molecular
Dynamics Study

Poster

M. Kozłowski, R. Kozubski,
J. Wróbel, T. Wejrzanowski,
K.J. Kurzydłowski, Ch. Goyhenex,
V. Pierron-Bohnes, M. Rennhofer,
S. Malinov
Atomic Ordering in Nano-Layered L10
AB Binaries: Multiscale Monte-Carlo
Simulations
Poster

G. Huang, F. Song
Modeling Dynamic Behavior of
Nanowires by Using a Semi-Continuum
Approach
Poster

I. Ladic, B. J. Thijsse
Self-healing of Aluminum Oxide Films:
Construction of a High-precision Al-O
Potential for Molecular Dynamics
Poster

R.C. Pasianot, V.P. Ramunni,
R.A. Pérez, M. Weissman,
J.R. Fernández
The Influence of Fe on the Zr Self-
diffusion: An Ab-initio Assessment
Poster

H. Löwe, J. Spiegel, B. Pinzer,
M. Schneebeli
Scale Dependent Micro-structural
Evolution of Snow
Poster

H. Seiner, O. Glatz, L. Bicanová,
P. Sedlák
Interfacial Microstructures in
Martensitic Transitions: From Optical
Observations to Mathematical Modeling
Poster

Z. Liu, H. Yu
Morphology Evolution of Stressed Fiber
due to Surface Diffusion
Poster

O. Englander
Nanostructure-Bulk Interfaces Formed
by Directed Self-Assembly
Poster

D. Stewart, Y. Osetsky, R. Stoller,
S. Golubov, B.-J. Lee, Y.-M. Kim
Atomistic Modeling of Screw
Dislocations in BCC iron: Inter-atomic
Potentials and Boundary Conditions
Poster

T. Takaki, Y. Hisakuni, A. Yamanaka,
Y. Tomita
Dynamic Recrystallization Simulation
by Phase - Field Method
Poster

L. Thuinet, A. Legris
Investigation of ζ Hydride Precipitation
in Zirconium
Poster

R. Oguma, S. Matsumura, T. Eguchi
Mesoscopic TDGL Model for
Microstructural Evolution of L10 Type
Ordering
Poster

M. P. Anisimov
Review of Nanomaterial Generation
From Vapor Phase
Poster

H. Kimizuka, H. Mori, S. Ogata
Phase-Field Modeling of Hydrogen-
Dislocation Interactions and its
Evolution in α -Iron
Poster

X. Xie
Micron-nanometer Lithium Manganese
Oxides
Poster

V. Fortov, O. Petrov, O. Vaulina
Dusty Plasma - MultiScale
Poster

Symposium 5
Computational materials design

Session M-B (Brent Adams, Chair)

Monday, 27 October 2008

Meeting Room A1

J. Wang, M. Li, J. Allison, P. D. Lee
Multiscale Modeling of the Influence of
Fe Content in a W319 Alloy on the
Distribution of Intermetallic Phases
and Micropores
10:20 a.m.

R. K. Mishra, K. Inal, O. Cazacu
Material Design through Multi-Scale
Simulations: Aluminum Sheet Forming
Using an Anisotropic Yield Function
Coupled with Crystal Plasticity Theory
10:50 a.m.

Y.-M. Kim, B.-J. Lee
Computational Design of Magnesium
Alloys for Improved Deformability
11:20 a.m.

D. Nguyen-Manh, S. L. Dudarev
A model tight-binding Hamiltonian
treatment of magnetic Fe-Cr alloys
11:40 a.m.

A. Kiejna, E. Wachowicz
Cohesion at Clean and Doped Grain
Boundaries in bcc Iron
12:00 p.m.

Session M-C (Byeong-Joo Lee, Chair)

Monday, 27 October 2008

Meeting Room A1

L. Zhang, L.-Q. Chen, Q. Du
Phase-field Prediction of Critical
Nucleus Morphology in Solids
1:40 p.m.

T. L. Tan, D. D. Johnson
Rapid And Accurate Estimate Of Alloy
Phase Transition Temperatures
2:20 p.m.

L. Xiong, Y. Chen
Modeling and simulations of
polycrystalline SiC thin film through a
coupled atomistic continuum theory
2:40 p.m.

Session M-D (Greg Olson, Chair)

Monday, 27 October 2008

Meeting Room A1

J.-C. Zhao, X. Zheng, D. Cahill
High-Throughput Measurements for
High-Fidelity Materials Databases for
Accelerated Materials Design
3:40 p.m.

B. L. Adams, B. S. Fromm, S. Ahmadi
Incorporating Grain Size Effects into
Microstructure Design
4:10 p.m.

M. Stan, B. Mihaila, D. Korzekwa,
P. Cristea, J. Ramirez
Computational Design of Advanced
Nuclear Fuels
4:40 p.m.

Session T-B (Peter D. Lee, Chair)

Tuesday, 28 October 2008

Meeting Room A1

C. Woodward, M. Groeber, M. Tschopp,
A. Rosenberger, D. Dimiduk, S. Russ
The Virtual Turbine Blade: Multi-
Length Scale Characterization of a
Single-Crystal Turbine Blade
10:20 a.m.

J. Neugebauer
Ab Initio Based Modeling of
Engineering Materials: From a
Predictive Thermodynamic Description
to Tailored Mechanical Properties
10:50 a.m.

C. Wu, S. V. Malinin, S. Tretiak,
V. Y. Chernyak
Electronic Excitations in Branched
Conjugated Molecules Using Exciton
Scattering Approach
11:20 a.m.

Y. V. Shtogun, L. M. Woods
Mechanically Altered Carbon Nanotubes
11:40 a.m.

Z.-K. Liu
Quantum, Statistic and Continuum
Thermodynamics of Material
12 :00 p.m.

Session T-C (J.C Zhao, Chair)
Tuesday, 28 October 2008
Meeting Room A1

J. Zimmermann, M. W. Finnis,
L. C. Ciacchi
Vacancy Segregation in the Initial
Oxidation Stages of the TiN(100)
Surface
1:40 p.m.

C. Qi, Y. Wang
Crystal Construction Based On Periodic
Surfaces
2:00 p.m.

B. Singh, O. Fritz
Computational modeling of materials for
electrical insulations
2:20 p.m.

D. Kilin, D. Micha
Density Matrix Treatment of
Confinement-Facilitated Photovoltage in
Thin Films of Silicon
2:40 p.m.

M. P. Anisimov, A. M. Baklanov,
A. V. Trilis
Nucleation Rate Surfaces for Modeling
of Nanomaterial Generation from
Crystals under Short Pulses of Energy
3:00 p.m.

Session W-B (Jörg Neugebauer, Chair)
Wednesday, 29 October 2008
Meeting Room A1

M. C. Gao, Ö. N. Doğan, P. King
Computational Design of Refractory
Alloys for Fossil Energy Applications
10:20 a.m.

V. Sundararaghavan
Multi-scale sensitivity analysis for
design of polycrystalline materials with
tailored properties
10:40 a.m.

S. A. Asgari, C. Yang, P. D. Hodgson,
B. F. Rolfe
Multiphase Material Modelling by
Multiscale Particle-In-Cell Method
11:00 a.m.

D. McDowell
Robust Simulation-Based Design of
Materials
11:20 a.m.

G.B.Olson
Systems Computational Design of
Hierarchically Structured Materials
11:50 a.m.

B. Brooks-Hinojosa, J. C. Nino,
A. Asthagiri
Computational Investigation of Bi
Containing Pyrochlores
12:20 p.m.

Session Th-D (Hamid Garmestani,
Chair)
Thursday, 30 October 2008
Meeting Room C

M. Khaleel
Design and Performance Modeling
Tools for Solid Oxide Fuel Cells
3:40 p.m.

D. Li, H. Garmestani
Computational Materials Design of Solid
State Fuel Cell Electrodes
4:00 p.m.

E. Lee, W. Cai, F. B. Prinz
Computing electrochemical impedance
of solid electrolyte from fluctuations
4:20 p.m.

Poster Session W-D (David McDowell
and Zi-Kui Liu, Chairs)
Wednesday, 29 October 2008
3:20-5:20 p.m.
Arena Access Area

X. Xie
Lithium and Zinc Composite Ceramic
Powders
Poster

R. J. Saffar
A Numerical Simulation to Relate the
Shot Peening Operation to the Induced
Residual Stresses of 15-5PH Steel
Poster

M. Katagiri, H. Onodera, H. Ogawa
Structural Stability of Hydrogen Storage
Materials

Poster

S. Ganopadhyay, T. Inerbaev,
A. E. Masunov, D. Altilio,
N. Orlovskaya, J. Mesit, R. Guha,
A. Sleiti, J. Kapat
Multiscale Simulations Combined
With Experimental Study of
Barium/Strontium Ferrate/Cobaltate
(BSCF) as a Promising Material For
Solid Oxide Fuel Cell (SOFC)

Poster

T.-E. Kim, Y.-S. Lee, W.-S. Jung,
S.-H. Chung, J.-H. Shim, J.-H. Choi,
S.-C. Lee
Electronic and Bonding Characteristics
of (Ti,Mo)C
Poster

S. Goel, A. E. Masunov
First Principles Study of Transition
Metal Diatomics as the First Step in
Multiscale Simulations of Carbon
Nanotube Growth Process
Poster

A. Ebrahimi, S. Jvdpour
Modeling Boring Operation in
Machining of Microalloyed and Heat-
Treated Alloy Steels for Study of
Machinability at Different Cutting
Condition
Poster

M. Ilkhani, M. R. Abolhassani,
S. J. Asadabadi
Electronic Structure and EFG
Calculation of CeIn₃ Under Pressure
Poster

Symposium 6
Multiscale modeling of radiation effects in materials

Session M-C (F. Willaime, Chair)

Monday, 27 October 2008

Meeting Room C

Joint Session with Symposium 9

D. Morgan, J. Tucker, T. Allen
Ab-initio Based Modeling of Diffusion and Radiation Induced Segregation in Ni-Fe-Cr alloys
1:40 p.m.

A. V. Barashev
Interaction of Interstitial Clusters With Solute Atoms in Ferritic Alloys and its Consequence for Microstructural Development Under Neutron Irradiation
2:10 p.m.

C. Domain, P. Olsson, E. Aublant, R. N. Happy, C. Becquart
An ab initio based AKMC model of ferritic Fe alloys Under irradiation
2:40 p.m.

M L Jenkins, Z. Yao, M. Hernandez-Mayoral, M. Kirk
Dynamic observations of heavy-ion damage in Fe and Fe-Cr alloys
3:00 p.m.

Session M-D (Syo Matsumura, Chair)

Monday, 27 October 2008

Meeting Room D

A. Caro, P. Erhart, B. Sadigh, G. Bonny, L. Malerba, M. Caro
The challenge to bridge scales in computational modeling Fe alloys
3:40 p.m.

T. T. Järvi, K. Nordlund, A. Kuronen, K. Albe
Ion irradiation of nanocrystals
4:10 p.m.

A. Badillo, R. Averback, P. Bellon
Microstructural Evolution of Binary Alloys under Irradiation
4:40 p.m.

Session T-C (Pascal Bellon and Dane Morgan, Chairs)

Tuesday, 28 October 2008

Meeting Room C

A. Chartier, T. Yamamoto, K. Yasuda, C. Meis, K. Shiiyama, S. Matsumura
Molecular dynamics simulation of irradiation induced phase transition in MgAl₂O₄
1:40 p.m.

Y. Chen, H.-Y. Geng, M. Iwasawa, Y. Kaneta, T. Ohnuma, M. Kinoshita
First principles modeling of defects behavior in UO₂ and CeO₂
2:10 p.m.

M. Yu. Lavrentiev, D. Nguyen-Manh, S.L. Dudarev
Magnetic Cluster Expansion Study of Magnetism and Thermodynamic Properties of Iron and Iron-Chromium Alloy
2:40 p.m.

D. Nguyen-Manh
Systematic Study of Interactions between Irradiated Defects and Impurities in Bcc Transition Metals
3:00 p.m.

Session T-D (S. Glubov and C. Domain,
Chairs)

Tuesday, 28 October 2008

Meeting Room D

Joint Session with Symposium 9

C A English, M L Jenkins
Molecular Ion Irradiations of
Molybdenum
3:20 p.m.

D. Stewart, Y. Osetsky, R. Stoller,
S. Golubov, T. Seletskaya, P. Kamenski
Atomistic studies of properties of helium
in BCC iron
3:40 p.m.

H. Heinisch
Atomic-scale Modeling of Helium
Atoms and Vacancies in Dislocations in
alpha-Iron
4:00 p.m.

F. Gao
Atomic-Level Modeling of Migration of
Vacancies, He Interstitials, and
Nucleation of He-V clusters at Grain
Boundaries in alpha-Fe
4:20 p.m.

R. Kurtz, H. Heinisch, F. Gao
Interaction of He_nV_m Clusters with
Coherent and Semi-Coherent Fe/Cu
Interfaces
4:40 p.m.

C. H. Woo
Resistance to Fast Dislocation Motion
5:00 p.m.

E. Martinez, J. Marian, A. Arsenlis,
M. Victoria, H.-J. Lee, B. Wirth
Combined Atomistic and Dislocation
Dynamics Modeling of Dislocation-SFT
Interactions in Cu
5:20 p.m.

Session W-C (Kai Nordlund, Chair)

Wednesday, 29 October 2008

Meeting Room B

L. Ventelon, F. Willaime, E. Clouet
Core Structure, Peierls Potential and
Kinks of Screw Dislocations in Iron
from First Principles
1:40 p.m.

W. J. Weber, F. Gao, R. Devanathan,
Y. Zhang, W. Jiang
Multiscale Modeling and Experimental
Validation of Radiation Effects in
Silicon Carbide
2:10 p.m.

D. Aidhy, T. Desai, P. Millett,
T. Watanabe, D. Wolf, S. Phillpot
Radiation Damage in Nanocrystalline
UO₂
2:40 p.m.

K. Shiyama, T. Yamamoto,
T. Takahashi, A. Guglielmetti,
A. Chartier, K. Yasuda, S. Matsumura,
K. Yasunaga, C. Meis
Molecular Dynamics Study of Frenkel
Pairs in Cerium Dioxide
3:00 p.m.

Session W-D (Rick Kurtz and D. Bacon,
Chairs)

Wednesday, 29 October 2008

Meeting Room D

Joint Session With Symposium 9

D. Rodney, T. Nogaret, M. Fivel
On the role of helical turns in the
formation of clear bands in irradiated
materials
3:20 p.m.

T. Tsuru, C. Suzuki, M. Yamaguchi,
Y. Kaji

Clustering process and precipitation hardening in Fe-Cu alloys: First-principle and empirical model evaluations
3:40 p.m.

Y. Osetskiy
Atomic-scale Modelling of Dislocation-obstacle Interactions in Irradiated Metals
4:00 p.m.

Y. Osetskiy
Dynamics of dislocation-localized obstacle interaction: what can we learn from atomic level modelling
4:20 p.m.

E. Clouet, S. Garruchet, H. Nguyen, M. Perez, C. Becquart
Dislocation interaction with C in α -Fe: a comparison between Atomic simulations and elasticity theory
4:40 p.m.

S. I. Golubov, B. N. Singh, M. Eldrup, A. M. Ovcharenko, R. E. Stoller
Study of Cavity Evolution in Iron under Neutron and α -Particle Irradiations
5:00 p.m.

A. Donev, V. V. Bulatov
First-passage Monte Carlo for materials under irradiation
5:20 p.m.

Session Th-B (Ying Chen and Alfredo Caro, Chairs)
Thursday, 30 October 2008
Meeting Room C

D. Schwen, M. Huang, R. S. Averback, P. Bellon
An Atomistic Study of Fission Gas Bubble Re-resolution in UO₂
10:20 a.m.

F. Gao, W. J. Weber, H. Y. Xiao, X. T. Zu
Ab initio Calculations of Defects, Defect Clusters and Defect Creation in SiC and GaN
10:40 a.m.

N. Castin, L. Malerba
New Approach To Model Point Defects Migration Using A Monte-Carlo Paradigm Coupled With Artificial Intelligence
11:00 a.m.

H. M. Urbassek, L. A. Sandoval
Influence of Electronic Stopping on Sputtering Induced by Cluster Impact on Metallic Targets
11:20 a.m.

D. Terentyev, M. H. Haghghat, R. Schäublin, L. Malerba
Interaction of dislocations with Cr-rich precipitates: a molecular dynamics study
11:40 a.m.

C. Deo, B. Uberuaga
Oxygen interstitial migration in hyperstoichiometric uranium dioxide studied by kinetic Monte Carlo simulations
12:00 p.m.

Poster Session W-D (Pascal Bellon and Fei Gao, Chairs)
Wednesday, 29 October 2008
3:20-5:20 p.m.
Arena Access Area

M. Okuniewski, C. Deo, J. Stubbins
Irradiation of helium implanted iron studied by multiscale modeling and experiments
Poster

G. Bonny, R. C. Pasianot, N. Castin,

L. Malerba
Fe-Cu-Ni many-body potential
consistent with thermodynamics
Poster

K. Morishita, Y. Watanabe, A. Kohyama,
H.L. Heinisch, F. Gao
KMC Simulations for Formation
Kinetics of Vacancy Clusters in beta-SiC
during Irradiation
Poster

Y. Watanabe, K. Morishita, A. Kohyama,
H.L. Heinisch, F. Gao, R. J. Kurtz
MD simulations for defect properties in
 β -SiC under irradiation – Energetics of
interstitial clusters
Poster

~~L. Zhang, M. Wei, L. Wu~~
~~The calculating analysis of the~~
~~relationship between specialities of~~
~~gamma spectrum and source condition~~
Poster

D. Terentyev, L. Malerba
Characterization of dislocation loops,
voids and Cr precipitates as competing
sources of hardening in irradiated
Fe-9Cr alloys
Poster

G. Lucas, R. Schäublin
Influence of helium on the clustering of
self-interstitials in irradiated bcc iron
Poster

Z. Chen, M. Mrovec, D. Weygand,
P. Gumbsch
Atomistic Modeling of the Interaction
between Dislocation and Vacancy in
Tungsten
Poster

K. Nakashima, N. Soneda, A. Nomoto
Kinetic Monte-Carlo simulation of
Irradiation Damage Accumulation in
Strain Field of Dislocation
Poster

T. Suzudo, M. Itakura, H. Kaburaki
Modeling Study of Grain Sub-division
Observed at High Burnup Nuclear Fuel
Poster

P. Olsson, C. Domain
Modelling of isochronal annealing in
bcc metals
Poster

Symposium 7
**Computational modeling of biological
and soft condensed matter systems**

Session M-B (Jeff Saven, Chair)

Monday, 27 October 2008

Meeting Room D

G. A. Voth
A Systematic Approach for Coarse-
graining Biomolecular and Soft Matter
Systems
10:20 a.m.

C. Matos, J. White, L. Hight, J. Burkett,
J. Wojtas, J. Cloud, J. Wilker
Characterizing and Mimicking Marine
Biological Materials: Recent
Experimental Results and Current Needs
for Modeling
10:50 a.m.

G. Mohan, D. Kopelevich
A Multi-Scale Model for Kinetics of
Formation and Disintegration Of
Spherical Micelles
11:20 a.m.

S. Yasuda, R. Yamamoto
A Model of Hybrid Simulations of MD
and CFD
11:40 a.m.

A. Chakrabarty, T. Cagin
Coarse Grain Modeling of Piezoelectric
Polyimide Copolymers
12:00 p.m.

Session M-C (Wei Yang, Chair)

Monday, 27 October 2008

Meeting Room D

D. Pochan
Construction of Nanostructures and
Materials through Peptide or Charged
Block Copolymer Self-assembly

1:40 p.m.

A. Liu, K.-C. Lee
New Proposed Mechanism for Actin-
Polymerization-Driven Motility
2:10 p.m.

J. Schneider, M. O. Steinhauser
Computational Modeling of Complex
Fluids – Scaling Properties of Flexible
and Semiflexible Polymer Chains
2:40 p.m.

L. C. Ciacchi, D. J. Cole, M. Koleini,
P. Gumbsch
Atomistic Modelling of Biomolecular
Adhesion on Materials Surfaces
3:00 p.m.

Session T-B (Darrin Pochan, Chair)

Tuesday, 28 October 2008

Meeting Room D

U.H.E. Hansmann
Simulating Folding and Interaction of
Proteins
10:20 a.m.

A. Warmflash, A. Dickson,
P. Bhimalapuram, A. R. Dinner
Umbrella Sampling For Non-
Equilibrium Processes
10:50 a.m.

W. Yang
Multi-Scale Sampling Design for
Biomolecular Simulations
11:20 a.m.

M. Paliy, R. Melnik, B. Shapiro
Forced Dynamics and Stability of RNA
Nanostructures
11:40 a.m.

S. P. Adiga, T. G. Desai

Dynamics of Polymers Adsorbed on Lipid Bilayers
12:00 p.m.

Session T-C (Jonathan Wilker, Chair)
Tuesday, 28 October 2008
Meeting Room D

C. Clementi
Prediction of Protein Functional States by Multi-Resolution Protein Modeling
1:40 p.m.

T. Truskett
Runniness and Randomness of Confined Fluids
2:10 p.m.

J. Saven
Engineering structure and function with theoretical protein design
2:40 p.m.

S. Tafur, K. Saponitsky, T. Inerbaev, A. Masunov
Multiscale modeling of non-linear optical materials for all-optical switching applications
3:00 p.m.

Poster Session T-D (Jeff Saven and Wei Yang, Chairs)
Tuesday, 28 October 2008
3:20-5:20 p.m.
Arena Access Area

S. Nikolov, C. Sachs, H. Fabritius, D. Raabe, M. Petrov, M. Friák, J. Neugebauer, L. Limperakis, D. Ma
Hierarchical Modeling of the Mechanical Properties of Lobster Cuticle from Nano- Up to Macroscale: The Influence of the Mineral Content and the Microstructure
Poster

P. Ghysels, G. Samaey, B. Tijkens, P. Van Liedekerke, H. Ramon, D. Roose
Application of Computational Homogenization to the Deformation of Biological Tissue
Poster

R. Yamamoto, T. Iwashita, Y. Nakayama, K. Kim
Direct Numerical Simulations for Electrokinetics of Colloids
Poster

L. Anisimova, M. P. Anisimov, P. K. Hopke
Computer Design of Water Vapor Nucleation Rate Surface
Poster

S. Kilina, S. Tretiak, D. Yarotski, A. Balatsky
Simulations of Electronic Properties of Self Assembled Soft Materials: DNA-adsorbents and Amorphous Polyfluorenes
Poster

S. Shanbhag
Self-diffusion in Binary Blends of Cyclic and Linear Polymers
Poster

R. Alapati, R. Devireddy, D. Moldovan
Hydrophilic pore formation in lipid bilayers in the presence of edgeactive agents: An atomistic simulation study
Poster

T. Murashima, T. Taniguchi
Multiscale Simulation for Rheological Phenomena
Poster

Q. Wang, T. Zhang
Modeling of Biofilm-Flow Interaction Using Kinetic Theories

Poster

C. Lu, S. Ni, W. Chen, C. Zhang
~~A Molecular Simulation~~
Study on Gas Transportation in
Poly(chloroparaxylene) Membrane
Poster

A. Meyer-Baese
Multi-Time Scale Deterministic and
Stochastic Analysis of the Heat Shock
Response System
Poster

G. Samaey
A Micro/Macro Approach for
Deformation of Biological Tissue
Poster

G.M. Shafiur Rahman, S. Itoh
A Study on Application of Underwater
Shock Wave for Jute Fiber Processing.
Poster

B. R. Novak, D. Moldovan,
G. L. Waldrop, M. S. de Queiroz
Umbrella Sampling Simulations of the
Closure of Biotin Carboxylase
Poster

Symposium 8 **Defects in materials**

Session M-D (Ladislav Kubin, Chair)
Monday, 27 October 2008
Meeting Room C

T. de la Rubia
Materials, Energy and Climate:
Requirements and Strategies for
Sustainability in the 21st Century
3:40 p.m.

M. Hribernik, G. R. Odette,
T. Yamamoto
On The Dynamics of Cleavage Fracture:
Atomic-Dislocation Scale Mechanisms
Leading to A Universal Toughness-
Temperature Shape
4:10 p.m.

L. P. W. Ma, C. H. Woo, S. L. Dudarev
Large-scale spin-lattice dynamics
simulation of ferromagnetic iron
4:40 p.m.

Session T-B (Elias Aifantis, Chair)
Tuesday, 28 October 2008
Meeting Room C

A. Takahashi, M. Kawanabe, S. Hayashi,
N. M. Ghoniem
Dislocation Dynamics Modeling of
Dislocation Cores in the Interaction with
Precipitates
10:20 a.m.

J. A. El-Awady, M. Wen,
N. M. Ghoniem
The Influence of Focused Ion Beam
Induced Damage on the Plasticity of
Nano- and Micro-pillars
10:40 a.m.

B.N Singh, S. Tähtinen

In-reactor Deformation Experiments on
FCC and BCC Pure Metals and Alloys
11:00 a.m.

L. P. Kubin, B. Devincre, T. Hoc
Scale Transitions in the Plasticity of
F.C.C. Single Crystals
11:20 a.m.

M. Zaiser, N. Nikitas, T. Hochrainer
Size Dependence in Constrained
Plasticity: Discrete and Continuous
Models of 3D Dislocation Dynamics
11:50 a.m.

Session W-B (Richard LeSar, Chair)
Wednesday, 29 October 2008
Meeting Room D

D. Walgraef, E. C. Aifantis
On the Gradient Theory of Elasticity and
Dislocation Dynamics
10:20 a.m.

R. Sedláček, J. Kratochvíl, C. Schwarz
Short-range Interactions in Continuum
Dislocation Plasticity
10:50 a.m.

I. Groma
Phase Field Theory of Dislocations
Obtained by Coarse Graining
11:20 a.m.

A. El-Azab
A Perspective on the Development of
Density-Based Models of Dislocation
Dynamics
11:40 a.m.

R. LeSar, J. Rickman
3D Simulations of Evolving Dislocation
Microstructures: Connection to Coarse
Graining
12:00 p.m.

H. Huang
A New Characteristic Length Scale
12:20 p.m.

Session W-C (Hanchen Huang, Chair)
Wednesday, 29 October 2008
Meeting Room D

T. Rahman
Self Learning Kinetic Monte Carlo
Simulations: application to hetero- and
homo-epitaxial growth processes
1:40 p.m.

K. Schwarz
Anomalous Relaxation in Strained (110)
fcc Layers
2:10 p.m.

E.H. Tan, L. Sun
Dislocation Dynamics Simulation in
Heterogeneous Elastic Thin Films
2:40 p.m.

M. Shehadeh, S. Banerjee, G. Lu,
N. Kioussis, N. Ghoneim
The Behavior of Dislocations in Bulk
and Nano-layered Crystals: An ab initio
based Parametric Dislocation Dynamics
Approach
3:00 p.m.

Session Th-B (Shahram Sharafat, Chair)
Thursday, 30 October 2008
Meeting Room A1

G. Ananthakrishna
Tracking Acoustic Emission and Spatial
Configurations of Dislocations during
the Portevin-Le Chatelier Effect
10:20 a.m.

J. S. Chen, X. Zhang, S. Osher
Meshfree Approaches for Modeling
Grain Structure Evolution
10:50 a.m.

A. Luque, J. Aldazabal,
J.M. Martínez-Esnaola, J. Gil Sevillano
Mode II Loading Behaviour of
Intergranular Cracks Lying on
Symmetrical Tilt Boundaries in Cu
11:20 a.m.

N. Kioussis, Z. Chen, N. Ghoniem
Local Chemistry Effect on Dislocation
Mobility: Sequential and Concurrent
Multi-scale Approaches
11:40 a.m.

Session Th-C (Steve Zinkle, Chair)
Thursday, 30 October 2008
Meeting Room A1

G. Lu
From electrons to finite elements:
quantum mechanical simulations at
macroscales
1:40 p.m.

P. Hirel, S. Brochard, J. Godet,
L. Pizzagalli
Study of dislocation nucleation
activation from surface step by atomistic
calculations
2:00 p.m.

R.C. Picu, R. Li, Z. Xu
Smooth Versus Jerky Motion of
Dislocations Across Fields of Obstacles
2:20 p.m.

M. Beneš, P. Strachota, Z. Čulík
Quantitative Aspects of Microstructure
Formation in Solidification
2:40 p.m.

Z. Wang, I. Beyerlein, R. LeSar
Material Deformation under High Rate:
Atomistic, Dislocation Dynamics
Simulations and Constitutive Modeling
3:00 p.m.

Session Th-D (Garani Ananthakrishna,
Chair)
Thursday, 30 October 2008
Meeting Room A1

S. Sharafat, A. Takahashi, K. Nagasawa,
N. Ghoniem
A Description of Helium Bubble Growth
in ODS Alloys using Monte Carlo
Simulation
3:40 p.m.

S. J. Zinkle, L. Wang
Defect Cluster Patterning in Irradiated
Materials
4:10 p.m.

S. B. Biner, Q. Chen, X-Y Liu
The Role of Solute Segregation on the
Evolution and Strength of Dislocation
Junctions
4:40 p.m.

Poster Session W-D (S. Noronha and S.
Sharafat, Chairs)
Wednesday, 29 October 2008
3:20-5:20 p.m.
Arena Access Area

D. Rodney, L. Proville
Why is the Peierls stress lower in
experiments than in simulations?
Poster

M.P. Anisimov, E.G. Fominykh,
A.B. Trilis
Experimental Measurements of
Nucleation Rates Near Critical
Conditions of Binary Vapor-Gas
Systems
Poster

V. Minárik, J. Kratochvíl, M. Beneš
Numerical Simulation of Dislocation
Dynamics – The Stress Field Evaluation
Threshold
Poster

J. Lao, D. Moldovan
Molecular Dynamics Simulation Study
of Pseudoelastic Effects in Palladium
Nanowires
Poster

C. Ayas, E. Van der Giessen
A Discrete Dislocation Approach to
Grain Boundary Diffusion
Poster

J. Godet, S. Brochard, T. Albaret,
L. Pizzagalli
Atomistic Calculations Of The
Formation, Stability And Mobility Of A
Non Dissociated 60° Dislocation In
Silicon
Poster

M. Perez, S. Garruchet
Coupling Molecular Dynamics and
Kinetic Monte-carlo Simulations to
Model the Carbon Snoek Peak in Ferrite
Poster

L. B. Zuev, S. A. Barannikova
A New Model of Plasticity Development
in Solids
Poster

H. Seddiki, M. Chabaat
2D-Stress analysis during crack-crazing
patterns interactions
Poster

S. Noronha, N. Ghoniem,
G. Ananthakrishna
A Dynamical for Flow Localization in
Irradiated Materials
Poster

Z. Chen, N. Kioussis, N. Ghoniem
Plarization-induced Strengthening
Mechanism of Cu Precipitate in alpha-Fe
Poster

Symposium 9
Elasticity to atomistics: predictive modeling of defect behavior

Session M-B (R. Stoller and Yu. Osetsky, Chairs)

Monday, 27 October 2008

Meeting Room C

R. Scattergood, S. Jang, Y. Purohit, D. Irving, D. Brenner
Molecular Simulations: Pb Segregation to Grain Boundaries and Effects on Deformation in Nanocrystalline Al.
10:20 a.m.

V. Vitek, R. Gröger
Modeling of Plastic Deformation of Non-magnetic Transition Body-Centered-Cubic Metals: From Atomic to Continuum Level
10:50 a.m.

R. C. Pond, J. P. Hirth
Dislocation Dynamics and Plasticity in Martensitic Transformations
11:20 a.m.

A. Serra, D. J. Bacon
Atomic Simulation of Twin Boundaries in HCP Metals: Mobility and Defect Interaction
11:40 a.m.

C. Brandl, E. Bitzek, P. M. Derlet, H. Van Swygenhoven
Dislocation activity within nanocrystalline metals: A molecular dynamics study
12:00 p.m.

Session M-C (F. Willaime, Chair)

Monday, 27 October 2008

Meeting Room C

Joint Session with Symposium 6

D. Morgan, J. Tucker, T. Allen
Ab-initio Based Modeling of Diffusion and Radiation Induced Segregation in Ni-Fe-Cr alloys
1:40 p.m.

A. V. Barashev
Interaction of Interstitial Clusters With Solute Atoms in Ferritic Alloys and its Consequence for Microstructural Development Under Neutron Irradiation
2:10 p.m.

C. Domain, P. Olsson, E. Aublant, R. N. Happy, C. Becquart
An ab initio based AKMC model of ferritic Fe alloys Under irradiation
2:40 p.m.

M L Jenkins, Z. Yao, M. Hernandez-Mayoral, M. Kirk
Dynamic observations of heavy-ion damage in Fe and Fe-Cr alloys
3:00 p.m.

Session T-D (S. Glubov and C. Domain, Chairs)

Tuesday, 28 October 2008

Meeting Room D

Joint Session with Symposium 6

C A English, M L Jenkins
Molecular Ion Irradiations of Molybdenum
3:20 p.m.

D. Stewart, Y. Osetsky, R. Stoller, S. Golubov, T. Seletskaya, P. Kamenski
Atomistic studies of properties of helium in BCC iron
3:40 p.m.

H. Heinisch
Atomic-scale Modeling of Helium
Atoms and Vacancies in Dislocations in
alpha-Iron
4:00 p.m.

F. Gao
Atomic-Level Modeling of Migration of
Vacancies, He Interstitials, and
Nucleation of He-V clusters at Grain
Boundaries in alpha-Fe
4:20 p.m.

R. Kurtz, H. Heinisch, F. Gao
Interaction of He_nV_m Clusters with
Coherent and Semi-Coherent Fe/Cu
Interfaces
4:40 p.m.

C. H. Woo
Resistance to Fast Dislocation Motion
5:00 p.m.

E. Martinez, J. Marian, A. Arsenlis,
M. Victoria, H.-J. Lee, B. Wirth
Combined Atomistic and Dislocation
Dynamics Modeling of Dislocation-SFT
Interactions in Cu
5:20 p.m.

Session W-C (V. Vitek and D. Rodney,
Chairs)

Wednesday, 29 October 2008

Meeting Room A1

D. Terentyev, D.J. Bacon,
P. Grammatikopoulos, Yu.N. Osetsky
Hardening by completely and partially
absorbed 1/2<111> and <100> dislocation
loops reacting with dislocations in α -Fe
1:40 p.m.

G. Monnet, Y. Osetsky, D. J. Bacon

Determination of the Activation Energy
of Dislocation-defect Interactions in
Molecular Dynamics Simulations
2:00 p.m.

C. Domain, G. Monnet
Molecular Dynamic Study of Screw
Dislocation – Irradiation Defect
Interactions
2:20 p.m.

L. Malerba, C. Becquart, C. Domain
Object kinetic Monte Carlo study of the
sink strength of dislocations
2:40 p.m.

M. Hou, A. Souidi, C. S. Becquart,
C. Domain, L. Malerba
A modelling study of the relationship
between primary damage features and
the long term defects clusters growth
3:00 p.m.

Session W-D (Rick Kurtz and D. Bacon,
Chairs)

Wednesday, 29 October 2008

Meeting Room D

Joint Session with Symposium 6

D. Rodney, T. Nogaret, M. Fivel
On the role of helical turns in the
formation of clear bands in irradiated
materials
3:20 p.m.

T. Tsuru, C. Suzuki, M. Yamaguchi,
Y. Kaji
Clustering process and precipitation
hardening in Fe-Cu alloys: First-
principle and empirical model
evaluations
3:40 p.m.

Y. Osetskiy
Atomic-scale Modelling of Dislocation-
obstacle Interactions in Irradiated Metals

4:00 p.m.

Y. Osetskiy
Dynamics of dislocation-localized
obstacle interaction: what can we learn
from atomic level modelling
4:20 p.m.

E. Clouet, S. Garruchet, H. Nguyen,
M. Perez, C. Becquart Dislocation
interaction with C in alpha-Fe: a
comparison between Atomic simulations
and elasticity theory
4:40 p.m.

S. I. Golubov, B. N. Singh, M. Eldrup,
A. M. Ovcharenko, R. E. Stoller
Study of Cavity Evolution in Iron under
Neutron and α -Particle Irradiations
5:00 p.m.

A. Donev, V. V. Bulatov
First-passage Monte Carlo for materials
under irradiation
5:20 p.m.

Session Th-C (R. Scattergood and A.
Serra, Chairs)
Thursday, 30 October 2008
Meeting Room D

A. Calder, D. Bacon, S. Barashev,
Y. Osetsky
Computer Simulation of Effects of PKA
Nature on Cascade Damage in Iron
1:40 p.m.

R. E. Stoller
Defect Production in Iron: Review of
Atomistic Simulations
2:00 p.m.

A. V. Barashev, S. I. Golubov,
D. J. Bacon, Y. N. Osetsky, R. E. Stoller

Decoration of Edge Dislocation with
Interstitial Clusters Under Neutron
Irradiation
2:20 p.m.

P. Gasca, C. Domain, A. Legris
Point defects in Zirconium and their
influence on radiation damage
2:40 p.m.

L. Ventelon, F. Willaime, E. Clouet
Core Structure, Peierls Potential and
Kinks of Screw Dislocations in Iron
from First Principles
3:00 p.m.

Session Th-D (B. Pond and G. Monnet,
Chairs)
Thursday, 30 October 2008
Meeting Room D

H. Trinkaus, B.N. Singh, S.I. Golubov
Mechanisms Operating during Plastic
Deformation of Metals
3:40 p.m.

V. Mohles, E. Jannot, G. Gottstein
On the role of elastic strains in the
precipitation of second phases
4:00 p.m.

S. Patinet
Substitutional Al solute interaction with
edge and screw dislocation in Ni: a
comparison between atomistic
computation and continuum elastic
theory
4:20 p.m.

L. Pillon, C. Denoual, Y.-P. Pellegrini
Influence of inertial effects on the
motion and the interaction of
dislocations
4:40 p.m.

PANELS

Session F-C

Friday, 31 October 2008

Meeting Room A-3

Panel I

11:00-11:40 a.m.

Future Directions in Multiscale
Materials Modeling

Panel II

11:40a.m.-12:20 p.m.

Applications of Multiscale
Materials Modeling