PROGRAM

International Conference on

MICROMECHANICS AND MICROSTRUCTURE EVOLUTION: MODELING, SIMULATION AND EXPERIMENTS

September 11 - 16, 2005
E. T. S. de Ingenieros de Caminos, Canales y Puertos
Ciudad Universitaria
Madrid, Spain

Conference chairs

S. B. Biner (Ames Laboratory, USDOE, USA)
J. Llorca (Polytechnic University of Madrid)
L. Kubin (LEM, CNRS- ONERA, France)
Y. Shibutani (Osaka University, Japan)
J. R. Morris (Oak Ridge National Laboratory, USDOE, USA)
G. Gottstein (Insitut fur Metallkunde, RWTH Germany)

ECI

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We wish to thank the following institutions for their support, which has been essential to the success of this conference:

- Spanish Ministry of Science and Education
- Polytechnic University of Madrid
- Office of Naval Research Global
- Acta Materialia
- Oak Ridge National Laboratory (USDOE)
- European Office of Aerospace Research and Development
- Air Force Office of Scientific Research
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D. J. Srolovitz
Y. Tomita
T. Ungar
H. van Swygenhoven
V. Vitek
S. Yip
SUNDAY, SEPTEMBER 11

17:00 – 19:00  Conference Check-In (Atocha Hotel)
19:00 – 20:00  ECI Welcome Reception

NOTES FOR CONFERENCE PARTICIPANTS

Participants should observe no smoking at ECI technical and social events.

During technical sessions please keep cell phones on vibrate or shut off. Take any telephone conversations out of the session room.

Presenters should leave time at the end of their talks for discussion and be available during breaks and meals for discussion.
### Session I:

**Opening session and Keynotes**

**Green Room**

- **08.45 - 08.50**  Welcome and announcements  
  Conference chairs

- **08.50 - 09.05**  Opening address by the Vice-Rector for Research of the Polytechnic University of Madrid

- **09.05 - 09.10**  Remarks by ECI Conferences Committee Chairman

- **09.10 - 09.40**  GEOMETRIC DESCRIPTION OF DEFECTS FROM THE NANO TO THE MACRO SCALE  
  N. M. Ghoniem and S. Banerjee

- **09.40 - 10.10**  UNIT CELL AND MEAN-FIELD MODELS OF DISCONTINUOUSLY-REINFORCED COMPOSITES  
  H. J. Böhm, A. Eckschlager, T. Drabek, D. Duschlbauer and H. E. Pettermann

- **10.10 - 10.30**  Coffee Break

### Session II-A:

**Chair** H. J. Böhm  
**Green Room**

- **10.30 - 10.50**  SIMULATION OF DUCTILE DAMAGE AND FRACTURE IN HETEROGENEOUS MATERIALS WITH A NONLOCAL DAMAGE MODEL  
  F. Reusch and B. Svendsen

- **10.50 - 11.10**  PLASTIC DEFORMATION OF COMPOSITE STRUCTURES IN CONTINUUM DISLOCATION-BASED APPROACH  
  R. Sedlacek, C. Schwarz and E. Werner

- **11.10 – 11.30**  THE MATERIAL POINT METHOD FOR MICROMECHANICS AND MICROSTRUCTURAL EVOLUTION IN POLYCRYSTALLINE MATERIALS  
  E. A. Holm, T. Bartel and M. Lusk (invited)

### Session II-B:

**Chair** N. M. Ghoniem  
**White Room**

- **10.30 - 10.50**  HIGH TEMPERATURE NANOINDENTATION FOR QUANTITATIVE STUDY OF DEFECT FORMATION  
  C. A. Schuh (invited)

- **10.50 - 11.10**  NONUNIFORMITY EFFECT OF NANOCRYSTALLINE MATERIALS IN NANO-INDENTATION AND MICROSCALE TENSILE TESTS  
  Y. Wei

- **11.10 - 11.30**  LARGE-SCALE ATOMISTIC SIMULATIONS OF NANOINDENTATION: LENGTH-SCALE EFFECTS ON HARDNESS  
  A. Hartmaier, X. Ma, S. Kilchert and H. Gao.

- **11.30 - 11.50**  Break
MONDAY, SEPTEMBER 12 (continued)

Session III-A:  
Chair  A. A. Benzerga  
Green Room
11.50 - 12.10  A COMPUTATIONAL MICROMECHANIC STUDY OF THE EFFECT OF THE INTERFACIAL PROPERTIES ON THE MECHANICAL BEHAVIOR OF THE COMPOSITE  
J. Llorca and J. Segurado

12.10 - 12.30  MODELING THE ROLE OF MICROSTRUCTURE ON SHEAR INSTABILITY WITH REFERENCE TO THE FORMABILITY OF AUTOMOTIVE ALUMINUM ALLOYS  
D. S. Wilkinson (invited)

12.30 - 12.50  CAPTURING MICROSTRUCTURAL SCALE EFFECTS THROUGH NONLOCAL CRYSTAL PLASTICITY  
C. C. Battaile, W. A. Counts, M. V. Braginsky and E. A. Holm.

Session III-B:  
Chair  T. Ohashi  
White Room
11.50 - 12.10  COMBINED EXPERIMENTAL AND SIMULATION ANALYSIS AT THE ATOMIC LEVEL OF DISLOCATION GENERATION AND MOBILITY AROUND NANO-INDENTATIONS IN AU(001)  
E. Carrasco, O. Rodriguez and J. M. Rojo

12.10 - 12.30  NANOINDENTATION ON CRYSTAL/AMORPHOUS POLYETHYLENE: A MOLECULAR DYNAMICS STUDY  
K. Yashiro, A. Furuta and Y. Tomita

12.30 - 12.50  DETAILED ASSESSMENT OF NANOINDENTATION SIZE EFFECTS IN RECRYSTALLIZED AND HIGHLY DEFORMED NIOBIUM  
J. Alkorta, J. M. Martinez and J. Gil-Sevillano

13.00 - 15.00  Lunch

Session IV:  
Keynotes  
Green Room
15.00 - 15.30  MULTISCALE MODELING OF FRACTURE  
W. A. Curtin, M. Dewald, V. Shastry and S. Qu

15.30 - 16.00  MULTIPLE SLIP DEFORMATION AND ACCUMULATION OF GEOMETRICALLY NECESSARY DISLOCATIONS IN METAL MICROSTRUCTURES UNDER NON-MONOTONIC EXTERNAL LOADING  
T. Ohashi and T. Inoue

16.00 - 16.20  Coffee Break
MONDAY, SEPTEMBER 12 (continued)

**Session V-A:** Chair *W. A. Curtin*  
*Green Room*

16.20 - 16.40 REVERSIBLE PLASTIC STRAIN IN THE CYCLIC LOADING–UNLOADING OF CAST MAGNESIUM ALLOYS: GRAIN SIZE, STRAIN AND SOLUTE EFFECTS  
C. H. Caceres, G. E. Mann, T. Sumitomo and J. Griffiths

16.40 - 17.00 MULTISCALE MODELLING OF FRACTURE OF FIBER-REINFORCED COMPOSITES  
C. González, C. de la Bastide, J. Segurado and J. LLorca

17.00 - 17.20 STRUCTURE-PROPERTY RELATIONSHIP IN METAL-MATRIX COMPOSITES  
A. Borbély, P. Kenesei and H. Biermann.

**Session V-B:** Chair *J. M. Martínez-Esnaola*  
*White Room*

16.20 - 16.40 MESOSCOPIC FINITE ELEMENT SIMULATIONS OF PYRAMIDAL INDENTATION EXPERIMENTS: CRYSTAL PLASTICITY ANALYSIS  
O. Casals, J. Ocenasek and J. Alcalá

16.40 - 17.00 AN AFM STUDY OF THE INITIAL STAGES OF PLASTICITY IN NANOINDENTED AU(111) AND AU(001) SURFACES  
A. Asenjo, M. Jafaar, V. Navarro, A. Mascaraque and J. M. Rojo

17.00 - 17.20 EVALUATION OF IN SITU MECHANICAL PROPERTIES OF ALUMINIUM MATRIX COMPOSITES BY NANOINDENTATION  
J. Rodríguez, P. Poza, T. Gómez and M. A. Garrido

17.45 Guided bus tour of the historical center of the city of Madrid.
TUESDAY, SEPTEMBER 13

Session VI:

**Keynotes**

08.55 - 09.00  Announcements

09.00 - 09.30  MULTI-DISLOCATION REACTIONS AND CRYSTAL PLASTICITY
V. V. Bulatov

09.30 - 10.00  DISCRETE DISLOCATION PLASTICITY ANALYSIS OF SIZE EFFECTS
IN SINGLE AND POLYCRYSTALS
V. S. Deshpande, A. Needleman and E. Van der Giessen.

10.00 - 10.20  Coffee Break

**Session VII-A:**  
**Chair** X. Markenscoff

10.20 - 10.40  LARGE-SCALE ATOMIC-LEVEL MODELING OF DISLOCATION-
OBSTACLE INTERACTIONS IN METALS
Y. Osetsky and D. Bacon (invited)

10.40 - 11.00  DISCONNECTIONS AS SOURCES OF TWINNING DISLOCATIONS IN
THE HCP METALS
A. Serra and D. J. Bacon

11.00 - 11.20  DISLOCATION DYNAMICS SIMULATIONS OF PRECIPITATION
HARDENING: APPLICATION ON IRRADIATION-INDUCED
PRECIPITATION OF NB NEEDLES IN A ZR-NB ALLOY
G. Monnet

11.20 - 11.40  SIZE EFFECTS UNDER HOMOGENEOUS DEFORMATION OF SINGLE
CRYSTALS: A DISCRETE DISLOCATION ANALYSIS
A. A. Benzerga and S. Guruzu

**Session VII-B:**  
**Chair** E. Oñate

10.20 - 10.40  THE MACROSCOPIC YIELD CRITERION FOR POROUS MATERIALS
WITH CUBIC SYMMETRY
A. Wilkins, T. Roberts and S. McElwain

10.40 - 11.00  MULTISCALE MODELLING OF COMPOSITE MATERIALS BY A
MULTIFIELD FINITE ELEMENT METHOD
P. Trovalusci, V. Sansalone and F. Cleri

11.00 - 11.20  MICROMECHANICAL PREDICTIVE MODEL OF AGEING
EMBRITTLEMENT OF DUPLEX STAINLESS STEELS
J. M. Alegre Calderon and F. Gutiérrez-Solana

11.20 - 11.40  EFFECT OF FIELD FLUCTUATIONS ON THE WORK-HARDENING OF
LINEAR POLYCRYSTALS AND COMPOSITES
O. Castelnau, R. Brenner and R. Lebensohn

11.40 - 12.00  Break
### TUESDAY, SEPTEMBER 13 (continued)

#### Session VIII-A:
- **Chair**: A. Serra
- **Green Room**

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<tr>
<td>12.00 - 12.20</td>
<td>DISLOCATION MICROSTRUCTURE, STRAIN LOCALISATION AND CRACK INITIATION IN FATIGUE STUDIED BY 3D DISCRETE DISLOCATION SIMULATIONS</td>
<td>M. C. Fivel, C. Depres and C. Robertson (invited)</td>
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<td>12.20 - 12.40</td>
<td>THE EFFECTIVE MASS OF A DISLOCATION IN A GENERAL MOTION</td>
<td>X. Markenscoff and L. Ni</td>
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<td>12.40 - 13.00</td>
<td>THE EFFECTS OF GRAIN SIZE ON THE STRENGTHENING BEHAVIOR OF POLYCRYSTALS: THE DISLOCATION DENSITY TENSOR APPROACH</td>
<td>S. B. Biner</td>
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#### Session VIII-B:
- **Chair**: D. Farkas
- **White Room**

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<td>MODELING OF CONCRETE FRACTURE AT MESO SCALE</td>
<td>R. C. Yu and G. Ruiz</td>
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<td>12.20 - 12.40</td>
<td>MODELLING OF PSEUDOELASTIC BEHAVIOUR IN CAST MAGNESIUM ALLOY AZ91</td>
<td>T. Sumitomo and C. Cáceres</td>
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<td>12.40 - 13.00</td>
<td>COUPLING DISCRETE METHODS AND FINITE ELEMENT METHODS FOR MULTISCALE STRUCTURAL ANALYSIS</td>
<td>E. Oñate, J. Rojek and C. Labra</td>
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13.00 - 15.00 Lunch

#### Session IX:
- **Keynotes**
- **Green Room**

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<td>FROM FOREST HARDENING TO STRAIN HARDENING IN FCC CRYSTALS: A DD SIMULATION STUDY</td>
<td>B. Devincre, L. Kubin and T. Hoc</td>
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<td>15.30 - 16.00</td>
<td>SYNERGIES BETWEEN SIMULATIONS AND EXPERIMENTS IN NC-METALS</td>
<td>H. Van Swygenhoven</td>
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<td>16.00 - 16.20</td>
<td>Coffee Break</td>
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<td>Time</td>
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<td>16.40 - 17.00</td>
<td>ANALYSIS OF THE STRENGTHENING CONTRIBUTIONS OF DISLOCATIONS AND BOUNDARIES IN A SEVERELY-PLASTICALLY-DEFORMED ALUMINUM ALLOY</td>
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<td>17.00 - 17.20</td>
<td>NON PLANAR CORE AND DYNAMIC EMISSION OF DISLOCATIONS IN FCC CRYSTALS</td>
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<td>17.20 - 17.40</td>
<td>SIMULATION OF MICROSTRUCTURE EVOLUTION IN POLycRYSTALLINE FERROELECTRICS-FERROELASTICS</td>
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<td>17.40 - 18.00</td>
<td>MULTI-SCALE POLycRYSTALLINE PLASTICITY SIMULATIONS FOR FCC AND BCC METALS AND ALLOYS USING FIELD THEORY-BASED UNIFIED CONSTITUTIVE MODEL</td>
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<td>16.40 - 17.00</td>
<td>DEFORMATION AND FRACTURE MECHANISMS IN NANOcRYSTALLINE METALLIC MATERIALS</td>
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<td>D. Farkas (invited)</td>
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<td>17.00 - 17.20</td>
<td>DISLOCATION NUCLEATION AT SURFACE NANOcRUCTURES</td>
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<td>G. Xu (invited)</td>
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<td>17.20 - 17.40</td>
<td>STRESS INTENSITY FACTOR IN NANOcRUCTURED SIC: AN ATOMIC SCALE INVESTIGATION</td>
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<td>L. Colombo, M. Ippolito, A. Mattoni and F. Cleri</td>
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<td>17.40 - 18.00</td>
<td>QUANTITATIVE PHASE FIELD MODELING OF EXTENDED DEFECTS USING AB INITIO CALCULATIONS AS INPUTS</td>
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<td>Y. Wang, C. Shen and J. Li (invited)</td>
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WEDNESDAY SEPTEMBER 14

**Session XI:**

08.55 - 09.00  Announcements  
09.00 - 09.30  3D DIGITAL MICROSTRUCTURES  
A. D. Rollett, D. Saylor, J. Fridy, A. Brahme, S. Lee, S. Sintay and R. Campman  
09.30 - 10.00  MULTISCALE APPROACHES TO MODELING PRECIPITATE MICROSTRUCTURE EVOLUTION IN ALLOYS  
L. Q. Chen  
10.00 – 10.20  Coffee Break

**Session XII-A:**

Chair **L. Q. Chen**  
10.20 - 10.40  ATOMISTIC MOLECULAR DYNAMICS MODELING OF IRRADIATION HARDENING IN FCC CRYSTALS  
T. Nogaret, C. Robertson and D. Rodney  
10.40 - 11.00  CORE EFFECTS IN MOLECULAR DYNAMICS SIMULATIONS OF DISLOCATIONS  
D. Rodney  
11.00 - 11.20  MOLECULAR DYNAMICS SIMULATION OF SCREW DISLOCATION MOTION IN BCC FE  
C. Domain and G. Monnet  
11.20 - 11.40  FLEXIBLE BOUNDARY CONDITION USING SPH METHOD FOR MOLECULAR DYNAMICS SIMULATION OF MATERIALS INTERFACE  
K. Saitoh

**Session XII-B:**

Chair **A. D. Rollett**  
10.20 - 10.40  GENERATING SELF-SIMILAR MICROSTRUCTURES IN STEELS. S. Das  
S. Verma, P. Saratha and M. Kadam  
10.40 - 11.00  DOMAIN GROWTH AND OFF-PHASE BOUNDARY STRUCTURES IN L12 TYPE ORDERING  
R. Oguma, T. Eguchi and S. Matsumura  
11.00 - 11.20  MESOSCOPIC SIMULATIONS ON THE EVOLUTION OF A SYSTEM OF DISLOCATIONS AND GRAIN BOUNDARIES  
H. Kaburaki, M. Itakura, T. Suzudo and S. Suzuki  
11.20 - 11.40  THE HOLE GROWTH AND COALESCENCE SIMULATIONS BY USING FEM AND CELLULAR AUTOMATA  
T. Tsuji and S. Katahira  
11.40 - 12.00  Break
**WEDNESDAY SEPTEMBER 14 (continued)**

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<td><strong>12.00 - 12.20</strong></td>
<td>MD SIMULATION OF DEFECT PRODUCTION DURING IRRADIATION OF NANOCRYSTALLINE MATERIALS</td>
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<td>M. Samaras, P. M. Derlet, H. Van Swygenhoven, W. Hoffelner and M. Victoria</td>
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<td><strong>12.20 - 12.40</strong></td>
<td>DISLOCATION INTERACTIONS WITH STACKING FAULT TETRAHEDRA: INSIGHT FROM ATOMISTIC MODELING AND IN SITU TEM DEFORMATION STUDIES</td>
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<td>H.-J. Lee, B. D. Wirth, J. Robach, I. M. Robertson and Y. Matsukawa</td>
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<td><strong>12.40 - 13.00</strong></td>
<td>ON META-DYNAMIC AND STATIC RECRYSTALLISATION OF NICKEL BASE ALLOYS</td>
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<td>C. Sommitsch, W. Mitter, P. Pélt and S. Kleber</td>
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<td><strong>12.00 - 12.20</strong></td>
<td>PREDICTION OF CASTING STRUCTURE FORMATION FOR ALUMINUM BASE ALLOYS USING CELLULAR AUTOMATON METHOD</td>
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<td>K. Ohsasa, T. Akagiri and K. Kurokawa</td>
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<td><strong>12.20 - 12.40</strong></td>
<td>DETERMINISTIC MODEL FOR ICE CREAM SOLIDIFICATION</td>
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<td>J. Aldazabal, A. Martín-Meizoso and J. M. Martinez</td>
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<td><strong>12.40 - 13.00</strong></td>
<td>DIFFUSION CREEP OF A TWO-PHASE POLycRYSTAL</td>
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<td>S. P. A. Gill</td>
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<td><strong>13.00 - 15.00</strong></td>
<td>Lunch</td>
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<td><strong>15.00 - 23.00</strong></td>
<td>Excursion to Toledo and conference banquet</td>
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<td>08.55 - 09.00</td>
<td>Announcements</td>
<td>DISCRETE DISLOCATION DYNAMICS</td>
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<td>M. Ortiz, A. Ramasubramanian and P. Ariza</td>
<td>DISCRETE DISLOCATIONS MODELING CRACK OPENING IN A BIMATERIAL</td>
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<td>S. Groh, A. Needleman and S. Kumar.</td>
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<td>09.00 - 09.30</td>
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<td>09.30 - 10.00</td>
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<td>10.00-10.20</td>
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**Session XV-A:**

**Chair:** J. Gil-Sevillano

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<td>10.20 - 10.40</td>
<td>SMALL-ANGLE NEUTRON SCATTERING AND RATE THEORY APPLIED TO NEUTRON-IRRADIATION-INDUCED CLUSTERING OF DEFECTS AND COPPER ATOMS IN IRON</td>
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<td>F. Bergner, A. Gokhman and A. Ulbricht</td>
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<td>10.40 - 11.00</td>
<td>TENSILE AND TORSIONAL DEFORMATION OF &lt;111&gt; AXIALLY ORIENTED COPPER NANOWIRES</td>
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<td>A. Luque, J. Aldazabal, J. M. Martinez- Esnaola and J. Gil</td>
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<td>11.00 - 11.20</td>
<td>IN-SITU STUDY ON SECOND PHASE FORMING PROCESS DURING ION IMPLANTATION INTO AL. H. Takahashi, H. Kinoshita W. Watanabe, F. Phillipp and R. Gotthardt</td>
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<td>11.20 - 11.40</td>
<td>THE ROLE OF DEFORMATION TWinning IN MICROSTRUCTURAL EVOLUTION IN COLD-ROLLED AUSTENITIC STEELS</td>
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**Session XV-B:**

**Chair:** J. M. Perlado

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<td>10.20 - 10.40</td>
<td>DUAL ROLE OF DEFORMATION-INDUCED GEOMETRICALLY NECESSARY DISLOCATIONS WITH RESPECT TO LATTICE PLANE MISORIENTATIONS AND/OR LONG-RANGE INTERNAL STRESSES</td>
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<td>H. Mughrabi (invited)</td>
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<td>10.40 - 11.00</td>
<td>INFLUENCE OF YTTRIUM SEGREGATION AT THE GRAIN BOUNDARIES ON THE SUPERPLASTIC BEHAVIOUR OF NANO-YTZP: THEORY AND EXPERIMENTS</td>
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<td>C. Garcia, E. Zapata-Solvas, D. Gómez and A. Domínguez</td>
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<td>11.00 - 11.20</td>
<td>DEFECT BEHAVIOURS IN BCC TRANSITION METALS: A MULTISCALE MODELLING STUDY</td>
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<td>D. Nguyen-Manh (invited)</td>
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<tr>
<td>11.20 - 11.40</td>
<td>TORSIONAL STIFFNESSES AND IDEAL TORSIONAL STRENGTH OF CARBON NANOTUBES</td>
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<td>D. C. Chrzan and E. Ertekin (invited)</td>
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<tr>
<td>11.40-12.00</td>
<td>Break</td>
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<td>Time</td>
<td>Session XVI-A</td>
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<td>12.00 - 12.20</td>
<td>Chair S. Groh</td>
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<thead>
<tr>
<th>Time</th>
<th>Session XVI-B</th>
<th>Topic</th>
<th>Authors</th>
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</thead>
<tbody>
<tr>
<td>12.00 - 12.20</td>
<td>Chair M. Ortiz</td>
<td>MICROSTRUCTURE SIMULATION OF RADIATION DAMAGE IN METALS USING IMPROVED KINETIC MONTECARLO DEFECTS DIFFUSION MODELING</td>
<td>J. M. Perlado, M. Victoria, C. Arévalo, E. Martínez, P. Cepas, G. Valverde, M. J. Cautela, J. Marian, D. Gómez-Brice and M. Hernández</td>
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13.00 - 15.00  Lunch

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<td>15.00 - 15.30</td>
<td>Keynotes</td>
<td>DEFORMATION AND FRACTURE OF METAL FOAMS</td>
<td>P. R. Onck</td>
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<tr>
<td>15.30 - 16.00</td>
<td></td>
<td>MICROSTRUCTURE AND DEFORMATION PHYSICS OF NANOCRYSALLINE MATERIALS BY MOLECULAR DYNAMICS SIMULATIONS</td>
<td>D. Wolf</td>
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<tr>
<td>16.00 - 16.20</td>
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<td>Coffee Break</td>
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### Session XVIII-A

**Chair**: D. Wolf  
**Green Room**

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<tr>
<th>Time</th>
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<tr>
<td>16.20 - 16.40</td>
<td>CHEMICALLY-CONTROLLED ATOMISTIC STUDY OF AGE HARDENING IN BINARY ALLOYS</td>
<td>J. Marian, A. Caro and B. Sadigh</td>
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<tr>
<td>16.40 - 17.00</td>
<td>MULTISCALE MODELING OF THE CONSTITUTIVE BEHAVIOR OF POROUS MATERIALS</td>
<td>J. Marian, A. Mota, J. Knap and M. Ortiz</td>
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<tr>
<td>17.00 - 17.20</td>
<td>MODELLING PRECIPITATION BY MESOSCOPIC CLUSTER DYNAMICS</td>
<td>J. Lepinoux</td>
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### Session XVIII-B

**Chair**: P. R. Onck  
**White Room**

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<tr>
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<tr>
<td>16.20 - 16.40</td>
<td>DISLOCATION PATTERNING: FROM DISCRETE DYNAMICS TO MESO-SCALE DESCRIPTION</td>
<td>B. Bakó and I. Groma</td>
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<td>16.40 - 17.00</td>
<td>A NOVEL APPROACH TO EVALUATION OF ELASTIC MODULUS OF HARD AND SUPERHARD MATERIALS USING SPM</td>
<td>A. Useinov</td>
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<td>17.00 - 17.20</td>
<td>MICRO- AND MACRO-SCALE INVESTIGATION OF THE “MORPHING” CAPABILITY OF HYBRID COMPOSITE SYSTEMS</td>
<td>D. Bollas, P. Pappas, J. Parthenios and C. Galiotis</td>
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<td>17.20 - 17.45</td>
<td>Break</td>
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<tr>
<td>17.45 - 20.00</td>
<td>Poster Session / Wine &amp; Cheese reception</td>
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<td>Session</td>
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<td>08.55-09.00</td>
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<td>XX-A</td>
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<td>XX-B</td>
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<td>10.30-10.50</td>
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<td>10.50-11.15</td>
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11.15 - 12.30   Closing arguments and roundtable discussion
12.30   Lunch and departure
POSTER SESSION

THURSDAY, SEPTEMBER 16, 17.45 - 20.00

P1 3-D DISLOCATION DYNAMICS SIMULATION OF POLycrystAl PLASTICITY
C. de Sansal, B. Devincre and L. Kubin

P2 SIMPLE EXPRESSIONS FOR THE NECKING INSTABILITY AND THE INCREASE OF DUCTILITY WITH STRAIN RATE
N. Argaman

P3 THE DYNAMICS OF GLIDE OF SCREW DISLOCATIONS IN BCC Fe: A MOLECULAR DYNAMICS APPROACH
J. Chaussidon, M. Fivel and D. Rodney

P4 INTERGRANULAR FRACTURE OF EMBRITTLED COPPER BICRYSTALS. D. González
J. Gil and J. M. Martínez-Esnaola

P5 DEVELOPMENT OF A BOND-ORDER TYPE INTERATOMIC POTENTIAL FOR Si-B SYSTEMS
T. Kumagai, S. Hara, S. Izumi and S. Sakai

P6 THE SIZE OF A STATISTICAL REPRESENTATIVE VOLUME ELEMENT. D. Trias, J. Costa
A. Turon and J. E. Hurtado

P7 MECHANICAL RESPONSE OF COMPACTED NANOMETRIC IRON. R. Rodríguez-Baracaldo
J. A. Benito, J. M. Cabrera and J. M. Prado

P8 DISCRETE DISLOCATION DYNAMICS SIMULATION ON STABILITY AND MECHANICAL PROPERTIES OF DISLOCATION CELL STRUCTURES
A. Semba, T. Hasebe and Y. Tomita

P9 CRYSTAL PLASTICITY MODELING OF BCC METALS FOR MULTI-SCALE SIMULATION
Y. Fujino, T. Hasebe and Y. Tomita

P10 THE NON-UNIQUENESS OF MECHANICAL PROPERTY EXTRACTIONS FROM INSTRUMENTED PYRAMIDAL INDENTATION EXPERIMENTS: DIMENSIONAL ANALYSIS AND FINITE ELEMENT SIMULATIONS
J. Alcalá and O. Casals

P11 SIMULATION OF C-N-V PRECIPITATION IN STEELS ALLOWING FOR LOCAL CONCENTRATION FLUCTUATIONS
J. Aldazabal and C. García-Mateo
P12 COMPUTER SIMULATION OF PHOTOCATALYTIC ACTIVITY OF Mn₂O₄ (M = Ca, Sr)
M. Katagiri, T. Sasaki, H. Onodera and T. Matsumoto

P13 COMPUTATIONAL STUDIES OF INTERGRANULAR STRESS CORROSION CRACK PROPAGATION AND THE ROLE OF BRIDGING LIGAMENTS
A. P. Jivkov, N. P. C. Stevens and T. J. Marrow

P14 HOMOGENIZATION APPLIED TO NON-LINEAR COMPOSITES WITH IMPERFECT CONTACT CONDITIONS

P15 ON FRACTALITY AND TOPOLOGY OF INTERGRANULAR CREEP FRACTURE SURFACES
Y. Kaim, P. R. Onck and E. Van der Giessen

P16 THE SIZE OF THE DEFORMATION MICROSTRUCTURE IN DISLOCATION PLASTICITY
J. Kratochvíl, M. Kruz and R. Sedl

P17 MECHANICAL BEHAVIOUR OF MICROSTRUCTURES: EFFECT OF THE SUBSURFACE MICROSTRUCTURE
G. Lionel

P18 EXPERIMENTAL SIMULATION OF NEUTRON IRRADIATION DAMAGE IN REACTOR PRESSURE VESSEL STEELS
M. F. Hashmi, S. J. Wu and H. X. Li

P19 STUDY OF AUSTENITE STRENGTHENING, PRECIPITATION STATE AND FERRITE GRAIN SIZE OF A Nb-MICROALLOYED STEEL BY MEANS OF HOT ROLLING SIMULATION TESTS
M. Gómez, S. F. Medina, J. I. Chaves and P. P. Gómez

P20 CRITICAL LENGTH SCALE FOR FRICTIONAL FLAW-TOLERANT ADHESION
H. Yao and H. Gao

P21 SIMULATION OF CROSS SECTIONAL NANOINDENTATION IN INTERCONNECT STRUCTURES WITH COHESIVE FRACTURE MODELS

P22 A MOLECULAR DYNAMICS STUDY ON THE EVOLUTION OF VOIDS IN URANIUM DIOXIDE

P23 THE ATOMIC SCALE ORIGIN OF CRACK RESISTANCE IN BRITTLE FRACTURE
L. Colombo, A. Mattoni and F. Cleri
P24 ANOMALOUS CREEP BEHAVIOR OF TZP-NI NANOCOMPOSITES
A. Morales-Rodríguez, C. Pecharromán, S. López-Esteban, F. Esteban, A. Bravo, D. Gómez-García, A. Domínguez, S. Moya and M. Jiménez

P25 SELF-SIMILAR FLUCTUATIONS IN DRY FRICTION DYNAMICS

P26 ON THE RELATIONSHIP BETWEEN THE ACTIVATION PARAMETERS AND THE STRAIN HARDENING PARAMETERS IN TWO TEMPERED MARTENSITIC STAINLESS STEEL
R. Bonade and P. Spatig

P27 CELLULAR AUTOMATON MODEL OF FISSION GAS BEHAVIOR IN NUCLEAR FUEL
T. Suzudo, M. Itakura and H. Kaburaki.


P29 INFLUENCE OF MATERIAL AND HOMOLOGOUS TEMPERATURE ON THE LIMITATION IN MICROSTRUCTURAL REFINEMENT AND STRENGTHENING DUE TO SEVERE PLASTIC DEFORMATION
V. Andreas, H. Martin and P. Reinhard

P30 MODELS FOR DEFECTS IN GRAPHENE SHEETS
A. Carpio and L. L. Bonilla

P31 THE STRAIN ENERGY AND ITS ROLE IN THE SHAPE EVOLUTION OF HYDRIDES
Y. Greenbaum, D. Barlam and R. Z. Shneck

P32 CONSIDERATION OF ANISOTROPY IN GRAIN BOUNDARY ENERGY AND MOBILITY IN RELATION WITH PRECIPITATES IN ABNORMAL GRAIN GROWTH IN FE3%SI
H. Afer, N. Rouag and R. Penelle

P33 BUILT DAMPERS FOR FAMILY HOMES VIA SMA: AN ANSYS COMPUTATION SCHEME INCLUDING THE MESOSCOPIC AND THE MICROSCOPIC EXPERIMENTAL ANALYSIS
V. Torra, A. Isalgue, P. Terriault and F. C. Lovey

P34 EFFECT OF REINFORCEMENT GEOMETRY ON PRECIPITATION OF POWDER METALLURGY Al 2009/SiC COMPOSITES
P. Rodrigo, A. Ureña, P. Poza and V. Utrilla

P35 FATIGUE AND ACTIVATION STRESS DEGRADATION OF NICKEL-TITANIUM SHAPE MEMORY ALLOY WIRES
P. Pappas, D. Bollas, J. Parthenios and C. Galiotis

P36 ON FATIGUE CRACK PROPAGATION OF ONE WAY-RAIL ROAD
K. Farhangdoost and M. Kavoosi
P37  BOUNDARY ELEMENT REPRESENTATION OF INTERFACIAL FORCES IN 3-D DISLOCATION DYNAMICS
    J. A. El-Awady, Q. Chen, S. B. Biner and N. Ghoniem

P38  DISCRETE MODEL OF DISLOCATION DYNAMICS AND CRYSTAL PLASTICITY
    M.P. Ariza and M. Ortiz