

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)

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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.

MONDAY, SEPTEMBER 12

<u>Session I:</u> 08.45 - 08.50	<u>Opening session and Keynotes</u> Welcome and announcements Conference chairs	<i><u>Green Room</u></i>
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	
<u>Session II-A:</u> 10.30 - 10.50	Chair H. J. Böhm SIMULATION OF DUCTILE DAMAGE AND FRACTURE IN HETEROGENEOUS MATERIALS WITH A NONLOCAL DAMAGE MODEL F. Reusch and B. Svendsen	<i><u>Green Room</u></i>
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)	
<u>Session II-B:</u> 10.30 - 10.50	Chair N. M. Ghoniem HIGH TEMPERATURE NANOINDENTATION FOR QUANTITATIVE STUDY OF DEFECT FORMATION C. A. Schuh (invited)	<i><u>White Room</u></i>
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
ATOMISTIC LEVEL OF DISLOCATION GENERATION AND MOBILITY
AROUND NANO-INDENTATIONS IN AU(001)
E. Carrasco, O. Rodríguez 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. Martínez 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. Shastri 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

<u>Session VI:</u> 08.55 - 09.00	Keynotes Announcements	<i><u>Green Room</u></i>
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	
<u>Session VII-A:</u> 10.20 - 10.40	Chair <i>X. Markenscoff</i> LARGE-SCALE ATOMIC-LEVEL MODELING OF DISLOCATION- OBSTACLE INTERACTIONS IN METALS Y. Osetsky and D. Bacon (invited)	<i><u>Green Room</u></i>
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	
<u>Session VII-B:</u> 10.20 - 10.40	Chair <i>E. Oñate</i> THE MACROSCOPIC YIELD CRITERION FOR POROUS MATERIALS WITH CUBIC SYMMETRY A. Wilkins, T. Roberts and S. McElwain	<i><u>White Room</u></i>
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 EMBRITTEMENT 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)

<u>Session VIII-A:</u> 12.00 - 12.20	Chair A. Serra DISLOCATION MICROSTRUCTURE, STRAIN LOCALISATION AND CRACK INITIATION IN FATIGUE STUDIED BY 3D DISCRETE DISLOCATION SIMULATIONS M. C. Fivel, C. Depres and C. Robertson (invited)	<u>Green Room</u>
12.20 - 12.40	THE EFFECTIVE MASS OF A DISLOCATION IN A GENERAL MOTION X. Markenscoff and L. Ni	
12.40 - 13.00	THE EFFECTS OF GRAIN SIZE ON THE STRENGTHENING BEHAVIOR OF POLYCRYSTALS: THE DISLOCATION DENSITY TENSOR APPROACH S. B. Biner	
<u>Session VIII-B:</u> 12.00 - 12.20	Chair D. Farkas MODELING OF CONCRETE FRACTURE AT MESO SCALE R. C. Yu and G. Ruiz	<u>White Room</u>
12.20 - 12.40	MODELLING OF PSEUDOELASTIC BEHAVIOUR IN CAST MAGNESIUM ALLOY AZ91 T. Sumitomo and C. Cáceres	
12.40 - 13.00	COUPLING DISCRETE METHODS AND FINITE ELEMENT METHODS FOR MULTISCALE STRUCTURAL ANALYSIS E. Oñate, J. Rojek and C. Labra	
13.00 - 15.00	Lunch	
<u>Session IX:</u> 15.00 - 15.30	Keynotes FROM FOREST HARDENING TO STRAIN HARDENING IN FCC CRYSTALS: A DD SIMULATION STUDY B. Devincre, L. Kubin and T. Hoc	<u>Green Room</u>
15.30 - 16.00	SYNERGIES BETWEEN SIMULATIONS AND EXPERIMENTS IN NC- METALS H. Van Swygenhoven	
16.00 - 16.20	Coffee Break	

TUESDAY, SEPTEMBER 13 (continued)

- Session X-A:** *Chair B. Devincere* *Green Room*
16.20 - 16.40 DISLOCATION STRUCTURE EVOLUTION IN DEFORMED ALUMINUM AND COPPER
P. Landau, R. Z. Shneck, G. Makov and A. Venkert
- 16.40 - 17.00 ANALYSIS OF THE STRENGTHENING CONTRIBUTIONS OF DISLOCATIONS AND BOUNDARIES IN A SEVERELY-PLASTICALLY-DEFORMED ALUMINIUM ALLOY
M. A. Muñoz-Morris, I. Gutiérrez-Urrutia and D. G. Morris
- 17.00 - 17.20 NON PLANAR CORE AND DYNAMIC EMISSION OF DISLOCATIONS IN FCC CRYSTALS
D. Mordehai
- 17.20 - 17.40 SIMULATION OF MICROSTRUCTURE EVOLUTION IN POLYCRYSTALLINE FERROELECTRICS-FERROELASTICS
A. Y. Belov and W. S. Kreher
- 17.40 - 18.00 MULTI-SCALE POLYCRYSTALLINE PLASTICITY SIMULATIONS FOR FCC AND BCC METALS AND ALLOYS USING FIELD THEORY-BASED UNIFIED CONSTITUTIVE MODEL
T. Hasebe
- Session X-B:** *Chair H. Van Swygenhoven* *White Room*
16.20 - 16.40 ON THE ROLE OF INTERFACES IN STRENGTH OF METALLIC, NANOLAYERED COMPOSITES
R. G. Hoagland, J. P. Hirth and A. Misra (invited)
- 16.40 - 17.00 DEFORMATION AND FRACTURE MECHANISMS IN NANOCRYSTALLINE METALLIC MATERIALS
D. Farkas (invited)
- 17.00 - 17.20 DISLOCATION NUCLEATION AT SURFACE NANOSTRUCTURES
G. Xu (invited)
- 17.20 - 17.40 STRESS INTENSITY FACTOR IN NANOSTRUCTURED SIC: AN ATOMIC SCALE INVESTIGATION
L. Colombo, M. Ippolito, A. Mattoni and F. Cleri
- 17.40 - 18.00 QUANTITATIVE PHASE FIELD MODELING OF EXTENDED DEFECTS USING AB INITIO CALCULATIONS AS INPUTS
Y. Wang, C. Shen and J. Li (invited)

WEDNESDAY SEPTEMBER 14

<u>Session XI:</u> 08.55 - 09.00	Keynotes Announcements	<u>Green Room</u>
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	
<u>Session XII-A:</u> 10.20 - 10.40	Chair L. Q. Chen ATOMISTIC MOLECULAR DYNAMICS MODELING OF IRRADIATION HARDENING IN FCC CRYSTALS T. Nogaret, C. Robertson and D. Rodney	<u>Green Room</u>
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	
<u>Session XII-B:</u> 10.20 - 10.40	Chair A. D. Rollett GENERATING SELF-SIMILAR MICROSTRUCTURES IN STEELS. S. Das S. Verma, P. Saratha and M. Kadam	<u>White Room</u>
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)

<u>Session XIII-A:</u> 12.00 - 12.20	Chair <i>J. Marian</i> MD SIMULATION OF DEFECT PRODUCTION DURING IRRADIATION OF NANOCRYSTALLINE MATERIALS M. Samaras, P. M. Derlet, H. Van Swygenhoven, W. Hoffelner and M. Victoria	<i>Green Room</i>
12.20 - 12.40	DISLOCATION INTERACTIONS WITH STACKING FAULT TETRAHEDRA: INSIGHT FROM ATOMISTIC MODELING AND IN SITU TEM DEFORMATION STUDIES H.-J. Lee, B. D. Wirth, J. Robach, I. M. Robertson and Y. Matsukawa	
12.40 - 13.00	ON META-DYNAMIC AND STATIC RECRYSTALLISATION OF NICKEL BASE ALLOYS C. Sommitsch, W. Mitter, P. Pélt and S. Kleber	
<u>Session XIII-B:</u> 12.00 - 12.20	Chair <i>C. González</i> PREDICTION OF CASTING STRUCTURE FORMATION FOR ALUMINUM BASE ALLOYS USING CELLULAR AUTOMATON METHOD K. Ohsasa, T. Akagiri and K. Kurokawa	<i>White Room</i>
12.20 - 12.40	DETERMIMISTIC MODEL FOR ICE CREAM SOLIDIFICATION J. Aldazabal, A. Martín-Meizoso and J. M. Martínez	
12.40 - 13.00	DIFFUSION CREEP OF A TWO-PHASE POLYCRYSTAL S. P. A. Gill	
13.00 - 15.00	Lunch	
15.00 - 23.00	Excursion to Toledo and conference banquet	

THURSDAY , SEPTEMBER 15

<u>Session XIV:</u> 08.55 - 09.00	Keynotes Announcements	<u>Green Room</u>
09.00 - 09.30	DISCRETE DISLOCATION DYNAMICS M. Ortiz, A. Ramasubramanian and P. Ariza	
09.30 - 10.00	DISCRETE DISLOCATIONS MODELING CRACK OPENING IN A BIMATERIAL S. Groh, A. Needleman and S. Kumar.	
10.00-10.20	Coffee Break	
<u>Session XV-A:</u> 10.20 - 10.40	Chair <i>J. Gil-Sevillano</i> SMALL-ANGLE NEUTRON SCATTERING AND RATE THEORY APPLIED TO NEUTRON-IRRADIATION-INDUCED CLUSTERING OF DEFECTS AND COPPER ATOMS IN IRON F. Bergner, A. Gokhman and A. Ulbricht	<u>Green Room</u>
10.40 - 11.00	TENSILE AND TORSIONAL DEFORMATION OF <111> AXIALLY ORIENTED COPPER NANOWIRES A. Luque, J. Aldazabal, J. M. Martínez- Esnaola and J. Gil	
11.00 - 11.20	IN-SITU STUDY ON SECOND PHASE FORMING PROCESS DURING ION IMPLANTATION INTO AL. H. Takahashi, H. Kinoshita W. Watanabe, F. Phillipp and R. Gotthardt	
11.20 - 11.40	THE ROLE OF DEFORMATION TWINNING IN MICROSTRUCTURAL EVOLUTION IN COLD-ROLLED AUSTENITIC STEELS K. Higashida and T. Morikawa	
<u>Session XV-B:</u> 10.20 - 10.40	Chair <i>J. M. Perlado</i> DUAL ROLE OF DEFORMATION-INDUCED GEOMETRICALLY NECESSARY DISLOCATIONS WITH RESPECT TO LATTICE PLANE MISORIENTATIONS AND/OR LONG-RANGE INTERNAL STRESSES H. Mughrabi (invited)	<u>White Room</u>
10.40 - 11.00	INFLUENCE OF YTTRIUM SEGREGATION AT THE GRAIN BOUNDARIES ON THE SUPERPLASTIC BEHAVIOUR OF NANO-YTZP: THEORY AND EXPERIMENTS C. García, E. Zapata-Solvas, D. Gómez and A. Domínguez	
11.00 - 11.20	DEFECT BEHAVIOURS IN BCC TRANSITION METALS: A MULTISCALE MODELLING STUDY D. Nguyen-Manh (invited)	
11.20 - 11.40	TORSIONAL STIFFNESSES AND IDEAL TORSIONAL STRENGTH OF CARBON NANOTUBES D. C. Chrzan and E. Ertekin (invited)	
11.40-12.00	Break	

THURSDAY, SEPTEMBER 15 (continued)

<u>Session XVI-A:</u> 12.00 - 12.20	Chair S. Groh MULTISCALE MODEL FOR THE STUDY OF PHASE SEPARATION IN ALLOYS WITH COHERENT ELASTIC MISFIT D. Perez and L. J. Lewis	<u>Green Room</u>
12.20 - 12.40	MICROTWISTS & NANODEFECTS: EXPERIMENTAL EVIDENCE AND MATHEMATICAL MODELLING A. DiCarlo, M. Monteferrante, P. Podio-Guidugli, V. Sansalone and L. Teresi	
12.40 - 13.00	MECHANICAL PROPERTIES OF ALUMINA/METAL INTERFACES: AB INITIO CALCULATIONS AND THE DEVELOPMENT OF AB INITIO DATABASE FOR MESOSCOPIC SIMULATIONS M. Kohyama, S. Tanaka, R. Yang, S. V. Dmitriev and Y. Hangai.	
<u>Session XVI-B:</u> 12.00 - 12.20	Chair M. Ortiz MICROSTRUCTURE SIMULATION OF RADIATION DAMAGE IN METALS USING IMPROVED KINETIC MONTECARLO DEFECTS DIFFUSION MODELING J. M. Perlado, M. Victoria, C. Arévalo, E. Martínez, P. Cepas, G. Valverde, M. J. Caturla, J. Marian, D. Gómez-Brice and M. Hernández	<u>White Room</u>
12.20 - 12.40	COMPUTATIONAL ANALYSIS OF THE RELATION BETWEEN MICROSTRUCTURE AND MECHANICAL PROPERTIES FOR HIGH SOLID LOADED COLLOIDAL SYSTEMS I. Schenker, F. Filser and L. J. Gauckler	
12.40 - 13.00	EFFECT OF INTERFACE STRUCTURE ON DISLOCATION INTERACTIONS WITH PRECIPITATES AND HE BUBBLES: INSIGHT FROM ATOMISTIC MODELING AND IN-SITU TEM DEFORMATION STUDIES B.D. Wirth, J.-H. Shim, H.-J. Lee, J. Young-Vandersall, J. Robach and I.M. Robertson	
13.00 - 15.00	Lunch	
<u>Session XVII:</u> 15.00 - 15.30	Keynotes DEFORMATION AND FRACTURE OF METAL FOAMS P. R. Onck	<u>Green Room</u>
15.30 - 16.00	MICROSTRUCTURE AND DEFORMATION PHYSICS OF NANOCRYSTALLINE MATERIALS BY MOLECULAR DYNAMICS SIMULATIONS D. Wolf	
16.00 - 16.20	Coffee Break	

THURSDAY, SEPTEMBER 15 (continued)

<u>Session XVIII-A:</u> 16.20 - 16.40	Chair <i>D. Wolf</i> CHEMICALLY-CONTROLLED ATOMISTIC STUDY OF AGE HARDENING IN BINARY ALLOYS J. Marian, A. Caro and B. Sadigh	<u>Green Room</u>
16.40 - 17.00	MULTISCALE MODELING OF THE CONSTITUTIVE BEHAVIOR OF POROUS MATERIALS J. Marian, A. Mota, J. Knap and M. Ortíz	
17.00 - 17.20	MODELLING PRECIPITATION BY MESOSCOPIC CLUSTER DYNAMICS J. Lepinoux	
<u>Session XVIII-B:</u> 16.20 - 16.40	Chair <i>P. R. Onck</i> DISLOCATION PATTERNING: FROM DISCRETE DYNAMICS TO MESO-SCALE DESCRIPTION B. Bakó and I. Groma	<u>White Room</u>
16.40 - 17.00	A NOVEL APPROACH TO EVALUATION OF ELASTIC MODULUS OF HARD AND SUPERHARD MATERIALS USING SPM A. Useinov	
17.00 - 17.20	MICRO- AND MACRO-SCALE INVESTIGATION OF THE “MORPHING” CAPABILITY OF HYBRID COMPOSITE SYSTEMS D. Bolas, P. Pappas, J. Parthenios and C. Galiotis	
17.20 - 17.45	Break	
17.45 - 20.00	Poster Session / Wine & Cheese reception	

FRIDAY, SEPTEMBER 16

<u>Session XIX:</u> 08.55 - 09.00	Keynotes Announcements	<u>Green Room</u>
09.00 - 09.30	MODELLING BASED ON TOMOGRAPHIC IMAGES E. Maire, J. Adrien, S. Youssef and R. Gaertner.	
<u>Session XX-A:</u> 09.30 - 09.50	Chair <i>D. S. Wilkinson</i> EXPERIMENTAL AND SIMULATION STUDIES ON NANOSTRUCTURAL FLUCTUATION IN A METALLIC GLASS SYSTEM S. Watanabe, H. Takahashi and N. Q. Lam	<u>Green Room</u>
09.50 - 10.10	CREEP DEFORMATION BEHAVIOR OF A MODEL METALLIC GLASS: A MOLECULAR DYNAMICS SIMULATION S. B. Biner	
10.10 - 10.30	FATIGUE CRACK GROWTH BEHAVIOR IN A ZR-BASED BULK AMORPHOUS ALLOY T. Nakasone, T. Iwasaki, S. Yoshida and H. Matsuo	
10.30 - 10.50	MICROMECHANICS OF ELASTIC-PLASTIC CONTACT ANALYSIS FOR ROUGH MATERIAL WITH SELF-AFFINE FRACTAL SURFACE J. S. Jeon, S. Hyun, and Y. S. Kim	
<u>Session XX-B:</u> 09.30 - 09.50	Chair <i>E. Maire</i> COHESIVE ZONE MODELING IN LAYERED STRUCTURES: DECOHESION AND CRACK ADVANCE IN DUCTILE LAYERS N. Broedling, A. Hartmaier and H. Gao	<u>White Room</u>
09.50 - 10.10	INFLUENCE OF AUSTENITE GRAIN SIZE ON RECRYSTALLISATION- PRECIPITATION INTERACTION IN A V-MICROALLOYED STEEL AND DETERMINATION OF RPTT DIAGRAMS BY MEANS OF HOT TORSION TESTS S. F. Medina, A. Quispe, M. Gómez and M. I. Vega	
10.10 - 10.30	LASER-BASED IMPULSIVE FRACTURE OF SILICA AND SILICON: IS A PURE MODE I MECHANISM CORRECT? P. Hess and A. Lomonosov	
10.30 - 10.50	INTERACTION BETWEEN SELF-INTERSTITIAL CLUSTERS AND EDGE DISLOCATION WITH $1/3\langle 11-20 \rangle$ BURGERS VECTOR IN ALPHA-ZIRCONIUM Z. Rong	
10.50 - 11.15	Coffee Break	

FRIDAY, SEPTEMBER 16 (continued)

Session XXI: Green Room

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 MIN_2O_4 (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
J. C. López-Real, R. Rodríguez, J. Bravo, R. Guinovart, F. J. Sabina, R. Martínez and G. A. Maugin
- 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
D. González, J. Molina, I. Ocaña, M. R. Elizalde, J. M. Sánchez, J. M. Martínez-Esnaola, J. Gil, D. Pantuso, B. Sun, G. Xu, B. Miner, J. He, J. Maiz and T. Scherban
- P22 A MOLECULAR DYNAMICS STUDY ON THE EVOLUTION OF VOIDS IN URANIUM DIOXIDE
H. Kaburaki, F. Shimizu, T. Kadoyoshi, T. Suzudo, M. Itakura and H. Kimizuka
- 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. Pecharromás, S. López-Esteban, F. Esteban, A. Bravo, D. Gómez-García, A. Domínguez, S. Moya and M. Jiménez
- P25 SELFSIMILAR FLUCTUATIONS IN DRY FRICTION DYNAMICS
M. Duarte, J. M. Molina, R. Prieto, E. Louis and J. Narciso
- 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.
- P28 CRITICAL PARTICLE SIZE FOR INTERFACIAL DEBONDING IN POLYMER NANOCOMPOSITES. G.-T. Wang, J. Chen, Z.-Z. Yu, Z. Huang and Y.-W. Mai.
- 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 AI 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. Kavosi

- 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