



E-MRS Spring Meeting 2001  
June 5 - 8, 2001

## **SYMPOSIUM A**

Computational Materials Science Across Time and  
Length Scales

### **Symposium Organizers:**

**H. Dreysé**, IPCMS – GEMME, Strasbourg, France

**L.T. Wille**, Florida Atlantic University, USA

**R. Nieminen**, University of Technology, Espoo, Finland

This symposium will be partially supported by the ESF Programme Ψk "Electronic structure calculations for elucidating the complex atomistic behaviour of solids and surfaces"

Papers will be published in Computational Materials Science

# E-MRS 2001 SPRING MEETING

## SYMPOSIUM A

Tuesday, June 5, 2001  
Mardi 5 juin 2001

Morning  
Matin

### Session I: Fundamental Issues

- A-I.1** 09:00 -Invited- BRIDGING BETWEEN MICRO- AND MACRO-SCALES OF MATERIALS BY MESOSCOPIC MODELS, **B.I. Lundqvist**, Department of Applied Physics, Goteborg University and Chalmers, 412 96 Göteborg, Sweden
- A-I.2** 09:30 LARGE-SCALE AB INITIO MODELLING OF DEFECTS IN PEROVSKITES: Fe IMPURITY IN SrTiO<sub>3</sub>, R.A. Evarestov<sup>(a)</sup> and E.A. Kotomin,<sup>(b,c)</sup> <sup>(a)</sup>Dept of Quantum Chemistry, St Petersburg Univ., St Peterhof, Russia, <sup>(b)</sup>Max-Planck-Insitut fuer Festkoerperforschung, Heisenbergstr.1, Stuttgart, Germany, <sup>(c)</sup>Institute of Solid State Physics, University of Latvia, Riga, Latvia
- A-I.3** 09:45 DIVACANCIES IN 3C- AND 4H-SiC, L. Torpo, T.E.M. Staab and R.M. Nieminen, Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, 02015 Hut, Finland
- A-I.4** 10:00 -Invited- MICROSTRUCTURE EVOLUTION FROM THE ATOMIC SCALE UP, **F. Cleri**, ENEA, Divisione Materiali, Centro Ricerche Casaccia, C.P.2400, 00100 Roma A.D., Italy
- 10:30 **BREAK**
- A-I.5** 11:00 BEYOND SHORT-RANGE ORDER LENGTH SCALS IN SISORDERED MATERIALS : FIRST PRINCIPLES MODELING OF SiSe<sub>2</sub>, M. Celino<sup>(a,b)</sup> and C. Massobrio<sup>(a)</sup>, <sup>(a)</sup>IPCMS, 23 rue du Loess, 67037 Strasbourg, France, <sup>(b)</sup>HPCNP-ENEA, Casaccia, 00100 Rome A.D., Italy
- A-I.6** 11:15 ATOMIC PROCESSES AT BONDED INTERFACES STUDIED BY EMPIRICAL MOLECULAR DYNAMICS, K. Scheerschmidt, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle/Saale, Germany
- A-I.7** 11:30 -Invited- HIERARCHICAL MODELLING OF PRECIPITATE INDUCED AGING IN STEELS, **S. Schmauder**, Staatliche Materialprüfungsanstalt (MPA) University of Stuttgart, Pfaffenwaldring 32, 70569 Stuttgart, Germany
- 12:00 **LUNCH**

**Tuesday, June 5, 2001**  
Mardi 5 juin 2001

**Afternoon**  
Après-Midi

**Session II: Growth I**

- A-II.1** 14:00 -Invited- MULTISCALE APPROACH FOR METAL THIN FILM GROWTH, **P. Vogl**, U. Hansen, Walter Schottky Institut and Physics Department, Technische Universität München, 85748 Garching, Germany
- A-II.2** 14:30 THEORY OF THE GROWTH MODE FOR A THIN METALLIC FILM ON AN INSULATING SUBSTRATE, **D. Fuks**, Dept Mat Engin, Ben Gurion University, Beer-Sheva 84305, Israel, S. Dorfman, Dept Phys, Technion Haifa, 32000 Israel, Y.F. Zhukovski and E.A. Kotomin, Inst Solid State Phys, Uni Latvia, Riga 1063, Latvia, and A. Marshall Stoneham, Dept Phys, Uni College, London WC1E 6BT, UK
- A-II.3** 14:45 GLASSY PHENOMENA IN STRAINED EPITAXY, **V.I. Tokar**, Institute of Magnetism, National Academy of Sciences, 36-b Vernadsky str., 03142 Kiev-142, Ukraine, H. Dreyssé, IPCMS-GEMME, 23 rue du Loess, 67037 Strasbourg, France
- A-II.4** 15:00 EXTENSIVE MONTE CARLO SIMULATIONS OF THIN METAL FILMS, **A.M. Cadilhe** and Marta M.D. Ramos, Departamento de física, Universidade do Minho, Largo do Paco, 4700-320 Braga, Portugal
- A-II.5** 15:15 GROWTH OF AU CLUSTERS ON AMORPHOUS  $Al_2O_3$ : EVIDENCE OF CLUSTER MOBILITY ABOVE A CRITICAL SIZE, **J. Carrey**, J.-L. Maurice, F. Petroff and A. Vaurès, Unité Mixte de Physique CNRS/THALES, 91404 Orsay, France
- 15:30 **BREAK**
- A-II.6** 16:00 -Invited- UNDERSTANDING THE GROWTH OF NANOCUSTER FILMS, **P. Jensen**, N. Combe and J.-L. Barrat, Département de Physique des Matériaux, UMR CNRS 5586, Université Claude Bernard Lyon-1, 69622 Villeurbanne Cedex, France
- A-II.7** 16:30 MULTISCALE SIMULATION OF CLUSTER GROWTH AND DEPOSITION PROCESSES BY DIRECT SIMULATION MONTE CARLO METHOD, H. Mizuseki, K. Hongo, **Y. Kawazoe**, Institute for Materials Research, Tohoku University, Sendai, Japan; L.T. Wille, Department of Physics, Florida Atlantic University, Boca Raton FL 33431, USA
- A-II.8** 16:45 DEPENDENCE OF PERIOD MACRO STRUCTURES ON KINETIC PARAMETERS UNDER DIRECTED CRYSTALLIZATION, **A. Gus'kov**, A. Orlov, Institute of Solid State Physics, Academy of Sciences of Russia, Moscow District, Chernogolovka 142432, Russia
- A-II.9** 17:00 INFLUENCING OF OSCILLATIONS OF AN EXTERNAL THERMAL FIELD ON PROCESS OF MICROSEGREGATION AT SINGLE CRYSTALS GROWTH BY A METHOD OF A DIRECTIONAL CRYSTALLIZATION, **A.A. Serov**, Zelenograd Scientific Research Center "Elsov", korp. 452, kv. 76, 103498 Moscow, Russia and V.M. Maslovsky, Zelenograd State Research Institute of Physical Problems, 103460 Moscow, Russia

**Wednesday, June 6, 2001**  
Mercredi 6 juin 2001

**Afternoon**  
Après-Midi

**Session III: Growth II**

- A-III.1** 14:00 -Invited- GROWTH MECHANISMS: FROM A MICROSCOPIC TO A MESOSCOPIC SCALE, **J. Neugebauer**, L. Mandreoli, M. Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft Faradayweg 4-6, 14195 Berlin, Germany, J.E. Northrup, Xerox Palo Alto Research Center 3333 Coyote Hill Road, Palo Alto CA 94304, USA
- A-III.2** 14:30 2-DIMENSIONAL MACROSCOPICAL SIMULATIONS OF POROUS SILICON GROWTH **G. Barillaro**, **P. Bruschi**, F. Pieri, Dipartimento di Ingegneria dell'Informazione, Università degli Studi di Pisa, via Diotisalvi 23 56126 Pisa, Italy
- A-III.3** 14:45 INTERACTION EFFECTS IN MAGNESIUM OXIDATION: A LATTICE-GAS SIMULATION, **E. Schröder**, Department of Applied Physics, Vasa 11, Chalmers University of Technology and Göteborg University, 41296 Gothenburg, Sweden
- A-III.4** 15:00 STUDY OF ION SCATTERING AND DECHANNELING FROM SURFACE DEFECT STRUCTURE BY COMPUTER SIMULATION, **H. Dreyse**, IPCMS, 23 rue du Loess, BP 20 CR, 67037 Strasbourg, France, **A.A. Dzhurakhalov**, Institute of Electronics, F. Khodjaev Str. 33, 700143 Tashkent, Uzbekistan, **B.S. Kalandarov**, **M. Kurbonov**, **U.O. Kutliev**, Urgench State University, 740000 Urgench, Uzbekistan
- A-III.5** 15:15 SELF-DIFFUSION ON Pd(111) BY MOLECULAR DYNAMICS SIMULATION, **N.I. Papanicolaou**, Department of Physics, Solid State Division, University of Ioannina, P.O. Box 1186, 45110 Ioannina, Greece
- A-III.6** 15:30 SIMULATION OF DIFFUSION UNDER PRESSURE, **A.V. Nazarov**, **M.G. Ganchenkova**, Dept. Materials Science, Moscow Engineering Physics Institute, 31 Kashirskoe shosse, 115409 Moscow, Russia, **A.A. Mikheev**, Department of Metal Physics, I.P. Bardin Central Research Institute of Ferrous Metallurgy, Moscow 107005, Russia
- A-III.7** 15:45 KINETIC MONTE CARLO-DYNAMIC RELAXATION METHOD: ZrO<sub>2</sub> FILM GROWTH MODELLING AND SIMULATION, **A.A. Knizhnik**<sup>(a)</sup>, **I.V. Belov**<sup>(a)</sup>, **A.A. Bagatur'yants**<sup>(a)</sup>, **B.V. Potapkin**<sup>(a)</sup> and **A.A. Korkin**<sup>(b)</sup>, <sup>(a)</sup>Kinetic Technologies Ltd, Moscow, Russia, <sup>(b)</sup>Semiconductor Products Sector, Motorola, Mesa AZ 85202, USA
- 16:00 **BREAK**
- 16:15 – 18:00 **Poster Session 1**

## Session IV: Poster session 1

- A-IV/P1.1** GRAPHITE AND MAGNESIUM HYDROGEN DYNAMICS, N. Jacobson, B. Tegner, H. Rydberg, P. Hyldgaard and B.I. Lundqvist, Department of Applied Physics, Chalmers University of Technology and Göteborg University, Sweden
- A-IV/P1.2** SOME ISSUES RELATED TO THE PARAMETERIZATION OF ELECTRONEGATIVITY EQUALIZATION METHODS, D. Mathieu and E. Germaneau, CEA-LR, BP 16, 37260 Monts, France
- A-IV/P1.3** TOPOGRAPHIC AND STRUCTURAL EVOLUTION OF ELECTROCHEMICAL ETCHED Si SAMPLES, G. Garozzo<sup>(a)</sup>, S. Coffa<sup>(b)</sup>, G. D'Arrigo<sup>(b)</sup>, A. La Magna<sup>(b)</sup>, C. Spinella<sup>(b)</sup>, M. Strobel<sup>(b,c)</sup>, <sup>(a)</sup>STMicroelectronics, Catania, Italy, <sup>(b)</sup>CNR-IMETEM, Catania, Italy, <sup>(c)</sup>IRIAM Center, University of Milan, Italy
- A-IV/P1.4** CALCULATION OF INTRINSIC STRESSES IN AMORPHOUS CARBON FILMS GROWN BY MOLECULAR DYNAMICS SIMULATION: FROM THE ATOMIC TO THE MACROSCOPIC SCALE, A.Yu. Belov and H.U. Jaeger, Forschungszentrum Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Postfach 510119, 01314 Dresden, Germany
- A-IV/P1.5** A NEW METHOD TO CALCULATE THE FRACTAL DIMENSION OF SURFACES: APPLICATION TO A MONTE CARLO DIFFUSION PROCESS ON A FRACTAL INTERFACE, M. Bigerelle and A. Iost, ESI, ENSAM Lille - LMPGM, CNRS UMR 8517, 8 Boulevard Louis XIV, 59046 Lille cedex, France
- A-IV/P1.6** PHASE SEPARATION IN THE SUPERSATURATED SOLID SOLUTIONS, T. Ischenko, General Physics Institute, Russian Academy of Sciences, Vavilov Street 38, 117942 Moscow, Russia
- A-IV/P1.7** INVESTIGATION OF THE DEFECT STRUCTURES SEMICONDUCTORS BY METHOD ION SCATTERING AT THE GRAZING INCIDENCE, U.O. Kutliev, F.F. Umarov, A.A. Dzhurakhalov, B.S. Kalandarov, M. Kurbanov, Urgench State University, Physical department, 740000 Urgench, Uzbekistan
- A-IV/P1.8** THE CONTROL OF THE DIAMETER OF A THIN FILAMENT, GROWN IN A VACCUUM BY E.F.G. METHOD, THROUGH THE CHANGE OF THE MELT TEMPERATURE AT THE MENISCUS BASIS, L. Braescu, University Politehnica Timisoara, Regina Maria str. 1, 1900 Timisoara, Romania, A.M. Balint and St. Balint, University of the West Timisoara, Blv. Parvan 4, 1900 Timisoara, Romania
- A-IV/P1.9** MODELING OF INFLUENCE OF SEMICONDUCTOR CRYSTAL NON-UNIFORMITIES UPON PARAMETERS OF RADIATION RESISTANT MAGNETIC FIELD SENSORS, L.A. Bolshakova, A.P. Bondarev, R.B. Tykhoniuk, Magnetic Sensor Laboratory, 1 Kotliarevsky St., 79013 Lviv, Ukraine
- A-IV/P1.10** SIMULATION OF DIFFUSION UNDER PRESSURE FOR DIFFERENT MECHANISMS IN B2 STRUCTURE, M.G. Ganchenkova, A.V. Nazarov, Dept. Materials Science, Moscow Engineering Physics Institute, 31 Kashirskoe shosse, 115409 Moscow, Russia
- A-IV/P1.11** THE CALCULATION OF ENERGETICAL PROFILE OF THE SHEAR IN THE ALLOYS WITH THE SUPERSTRUCTURE D019, M.A. Baranov, V.V. Romanenko, E.V. Chernyh, M.D. Starostenkov, Altai Technical State University, General Physics, Lenina Street 46, 656099 Barnaul, Russia
- A-IV/P1.12** SIMULATION OF ORDERING PROCESSES IN THIN FILMS OF THE ALLOY Cu<sub>3</sub>Au, M.D. Starostenkov, E.A. Dudnik, G.M. Poletaev, Altai Technical State University, General Physics, Lenina Street 46, 656099 Barnaul, Russia

- A-IV/P1.13** THE STABILITY OF THE PLANAR DEFECTS IN HCP ALLOYS, M.D. Baranov, E.V. Chernyh, M.D.Starostenkov, Altai Technical State University, General Physics, Lenina Street 46, 656099 Barnaul, Russia
- A-IV/P1.14** STRUCTURE OF NANOCRISTALIC DIAMONDS, M.D. Starostenkov, I.V. Loschina, Altai Technical State University, General Physics, Lenina Street 46, 656099 Barnaul, Russia
- A-IV/P1.15** A SIMPLE MODEL OF STRUCTURAL DISORDER IN III-V TERNARY ALLOYS, A.A. Kopylov, State Inst. of Metrology, PO Box 128, 196135, St.Petersburg, Russia, I.I. Parfenova, State Electrotech. Univ. (LETI), 197376, St.Petersburg, Russia
- A-IV/P1.16** ELECTRICAL PROPERTIES OF MONOCRYSTALLINE CdTe SURFACE, G. Khlyap, State Pedagogical University, 24 Franko str., Drogobych 82100, Ukraine
- A-IV/P1.17** MAGNETIC BEHAVIOR OF STRAINED Fe on Ir(001), N. Baadji, K. Louzazna and A. Haroun, Departement de physique, Université Ferhat Abbas, 19000 Sétif, Algeria

Thursday, June 7, 2001  
Jeudi 7 juin 2001

Morning  
Matin

**Session V: Elasticity**

- A-V.1** 09:00 -Invited- MECHANICAL PROPERTIES OF SINGLE CRYSTALS: MULTISCALE MODELLING, **L.P. Kubin**, LEM, CNRS-ONERA, 29 Av. de la Division Leclerc, BP 72, 92322 Chatillon Cedex, France
- A-V.2** 09:30 FROM AB-INITIO TO ELASTIC THEORY ANALYSIS: THE 90° PARTIAL DISLOCATION IN DIAMOND, **X. Blase**<sup>(a,d)</sup>, K. Lin<sup>(b,c)</sup>, A. Canning<sup>(c)</sup>, S.G. Louie<sup>(b,c)</sup>, D.C. Chrzan<sup>(c,d)</sup>, <sup>(a)</sup>Département de Physique des Matériaux and CNRS, Villeurbanne, France, <sup>(b)</sup>Department of Physics, University of California, Berkeley CA, USA, <sup>(c)</sup>Material Science Division, LBL, Berkeley CA, USA, <sup>(d)</sup>Department of Material Science, University of California, Berkeley CA, USA
- A-V.3** 09:45 THE MULTIPLE ATOMIC CONFIGURATIONS OF THE EDGE THREADING DISLOCATIONS IN GaN, **J. Chen**, A. Béré\*, P. Ruterana, A. Serra\* and G. Nouet, ESCTM-CRISMAT, Institut des Sciences de la Matière et du Rayonnement, 6 Bd Maréchal Juin, 14050 Caen Cedex, France, \*UPC, Departament de Matematica Aplicada III, Barcelona, Spain
- A-V.4** 10:00 -Invited- PLASTICITY ASSOCIATED WITH DYNAMIC FRACTURE: ATOMISTIC AND MULTISCALE SIMULATIONS, **R.E. Rudd**, James F. Belak, Lawrence Livermore National Laboratory, USA
- 10:30 **BREAK**
- A-V.5** 11:00 -Invited- FROM DISLOCATION CORE STRUCTURES TO INTERACTIONS, **K.W. Jacobsen**, CAMP, Dept. of Physics, DTU, Building 307, 2800 Kgs. Lyngby, Denmark
- A-V.6** 11:15 COMPUTER MODELS OF CRACK PATHS IN POLYCRYSTALLINE MATERIALS, W. Sychalski and **K.J. Kurzydowski**, Department of Materials Science and Engineering, Warsaw University of Technology, 02-524 Warszawa, Woloska 144, Poland
- A-V.7** 11:45 MECHANISMS OF DISLOCATION NUCLEATIONS AND DISLOCATION COMPLEXES IN THIN FILMS, **M.D. Starostenkov**, G.M. Poletayev, A.A. Ovcharov, Altai State Technical University, Barnaul, Russia
- 12:00 **LUNCH**

Thursday, June 7, 2001  
Jeudi 7 juin 2001

Afternoon  
Après-midi

### Session VI: Magnetism

- A-VI.1** 14:00 -Invited- MICROMAGNETIC SIMULATION OF THE MAGNETIC SWITCHING BEHAVIOUR OF MESOSCOPIC AND NANOSCOPIC STRUCTURES, **J. Fidler**, T. Schrefl, D. Suess, W. Scholz and V. Tsiantos, Institute of Applied and Technical Physics, Vienna University of Technology, Austria
- A-VI.2** 14:30 A NEW TECHNIQUE FOR FERROMAGNETIC RESONANCE CALCULATIONS, **J.C. Toussaint**<sup>(a)</sup>, A. Marty<sup>(b)</sup>, N. Vukadinovic<sup>(c)</sup>, J. Ben Youssef<sup>(d)</sup>, M. Labrune<sup>(e)</sup>,  
<sup>(a)</sup>Laboratoire Louis Néel, CNRS, 38042 Grenoble cedex 9, France, <sup>(b)</sup>CEA-Grenoble, Département de Recherche Fondamentale sur la Matière Condensée/SP2M, 38054 Grenoble cedex 9, France, <sup>(c)</sup>DTA/EM Dassault Aviation, 92552 Saint-Cloud, France, <sup>(d)</sup>Laboratoire de Magnétisme de Bretagne, CNRS-UPRES-A 6135, 29285 Brest, <sup>(e)</sup>Laboratoire LPMTM, Institut Galilée, Université Paris-13, 93430 Villetaneuse, France
- A-VI.3** 14:45 INVESTIGATION OF 3D MICROMAGNETIC CONFIGURATIONS IN CIRCULAR NANOELEMENTS, **L.D. Buda**, I.L. Prejbeanu, U. Ebels, K. Ounadjela, IPCMS - GEMME, 23 rue du Loess, 67037 Strasbourg, France
- A-VI.4** 15:00 EPITAXIAL GROWTH REGIMS AND CORRELATIONS BETWEEN MAGNETIC AND CHEMICAL STRUCTURES, **V.M. Uzdin**, Saint-Petersburg State University, ICAPE, V.O. 14 linia 29, St. Petersburg 199178, Russia
- A-VI.5** 15:15 LDA+U CALCULATED ELECTRONIC AND STRUCTURAL PROPERTIES OF NiO(001) AND NiO(111) P(2X2) SURFACES, **O.M. Bengone**, Dept. of Physics, Uppsala University, Box 530 751 21 Uppsala, Sweden, M. Alouani, IPCMS-GEMM, UMR 7504 du CNRS, Université Louis Pasteur, 23 rue du Loess, 67037 Strasbourg, France, J. Hugel, IPC-LPLI, 1 Bd Arago, 57078, Metz cedex3, France, P.E. Bloechl, Institute of Theoretical Physics, Clausthal University of Technology, Leibnizstr. 10, 38678 Clausthal-Zellerfeld, Germany
- A-VI.6** 15:30 INTERFACE ALLOYING AND MAGNETIC ORDERING FORMATION IN MULTILAYERS, **N.S. Yartseva**, S.V. Yartsev, Institute of Metal Physics, 620219 Ekaterinburg, Russia, V.M. Uzdin, ICAPE, St. Petersburg State University, 14 linia V.O. 29, St. Petersburg, Russia, C. Demangeat, IPCMS, 23 rue du Loess, 67037 Strasbourg Cedex, France
- A-VI.7** 15:45 FORMATION OF MAGNETIC CHARACTERISTICS AND HYPERFINE FIELD IN ALLOYS METAL-METALLOID, **A.K. Arzhnikov**, L.V. Dobysheva, Physical-Technical Institute of Ural Branch of Russian Academy of Sciences, Kirov str., 132, Izhevsk 426001, Russia
- 16:00 **BREAK**
- 16:15 – 18:00 **Poster Session 2**

## Session VII: Poster session 2

- A-VII/P2.1** QUANTUM MOLECULAR DYNAMICS SIMULATIONS OF CONJUGATED POLYMERS, A.M. Almeida, Marta M.D. Ramos and A.M. Cadilhe, Departamento de fisica, Universidade do Minho, Largo do Paco, 4700-320 Braga, Portugal
- A-VII/P2.2** MAGNETO-OPTICAL PROPERTIES OF IRON THIN FILMS ON PARAMAGNETIC SUBSTRATES, A. Debernardi, I. Galamakis, M. Alouani, and H. Dreyssé, Institut de Physique et Chimie des matériaux de Strasbourg, 23 rue du Loess, 67037 Strasbourg France
- A-VII/P2.3** CHARACTERIZATION OF THE DIFFUSION BY THE DATA COMPRESSION, M. Bigerelle and A. Iost. ESI, ENSAM Lille - LMPGM, CNRS UMR 8517, 8 Boulevard Louis XIV, 59046 Lille Cedex, France
- A-VII/P2.4** MODELING OF ZrO<sub>2</sub> DEPOSITION FROM ZrCl<sub>4</sub> AND H<sub>2</sub>O ON THE Si(100) SURFACE: INITIAL REACTIONS AND SURFACE STRUCTURES, V.V. Brodskii<sup>(a)</sup>, E.A. Rykova<sup>(a)</sup>, A.A. Bagatur'yants<sup>(a)</sup> and A.A. Korkin<sup>(b)</sup>, <sup>(a)</sup>KINETIC TECHNOLOGIES Ltd, Moscow, Russia, <sup>(b)</sup>Semiconductor Products Sector, Motorola, Mesa AZ 85202, USA
- A-VII/P2.5** MODELING AND SIMULATION OF Be DIFFUSION IN InP/InGaAs METAL HETEROJUNCTION BIPOLAR TRANSISTOR, M. Ihaddadene<sup>(a)</sup>, J.Marcon<sup>(a)</sup>, M. Idrissi-Benzohra<sup>(a)</sup>, K.Ketata<sup>(a)</sup>, M.Ketata<sup>(a)</sup>, S.Demichel<sup>(b)</sup> and J-L.Pelouard<sup>(b)</sup>, <sup>(a)</sup>LEMI-IUT, Université de Rouen, 76821 Mont Saint Aignan, France, <sup>(b)</sup>L2M-CNRS, 196 Av. H. Ravéra, 92225 Bagneux Cedex, France
- A-VII/P2.6** THE INVESTIGATION OF THE ION REFOCUSING EFFECT ON THE SURFACE Cu(100) AT DIFFERENT CRISTALLOGRAFIC DIRECTIONS, U.O. Kutliev, A.A. Dzhurakhalov\*, B.S. Kalandarov, M.K. Kurbanov, Urgench State University, Urgench, Uzbekistan, \*Institute of Electronics, Uzbek Academy Science, Tashkent, Uzbekistan
- A-VII/P2.7** ATOMISTIC AND CONTINUUM STUDIES OF CARBON NANOTUBES UNDER PRESSURE, P.S. Das, ColTec Inc., Columbus IN 47201, USA and L.T. Wille, Department of Physics, Florida Atlantic University, Boca Raton FL 33431, USA.
- A-VII/P2.8** THE DOPANT DISTRIBUTION COMPUTED IN THE MODIFIED CHANG-BROWN MODEL IN QUASI-STEADY STATE APPROXIMATION, M.M. Mihailovici, A.M. Balint and St. Balint, University of the West Tmisoara, Blv. Parvan 4, 1900 Timisoara, Romania
- A-VII/P2.9** MODELING OF PHYSICAL-CHEMICAL PROCESSES OF GROWTH AND COMPLEX DOPING FOR SEMICONDUCTOR MICROCRYSTALS, L.A. Bolshakova, I.I. Melnyk, T.A. Moskovets, P.S. Koptsev, Magnetic Sensor Laboratory, 1 Kotliarevsky St., 79013, Lviv, Ukraine
- A-VII/P2.10** STRUCTURE-ENERGETICAL TRANSFORMATIONS AT COMBUSTION SYNTHESIS IN THE SYSTEMS NiAl AND TiAl, M.D. Starostenkov, G.M. Poletayev, A.G. Starostenkova, Altai Technical State University, General Physics, Lenina Street 46, 656099 Barnaul, Russia
- A-VII/P2.11** INFLUENCE OF A MISORIENTATION ANGLE ON AN ENERGY OF THE GRAIN BOUNDARY M.D. Starostenkov, B.F. Demyanov, A.V. Weckman, Altai Technical State University, General Physics, Lenina Street 46, 656099 Barnaul, Russia
- A-VII/P2.12** DEFORMATION AI OF TRANSFORMATION OF THE STRUCTURE 3D CRYSTAL AI, CONTAINING BLUNTED CRACK Gorge N. Y., M.D. Starostenkov, G.M. Poletayev, Altai Technical State University, General Physics, Lenina Street 46, 656099 Barnaul, Russia
- A-VII/P2.13** COMPUTER SIMULATION OF THE DEFECT STRUCTURE FORMATION IN CRYSTAL LATTICES BY LOW-ENERGY ION IRRADIATION, I.V. Tereshko, V.I. Khodyrev, B.B. Glushchenko, A.M. Tereshko, The Mogilev State Technical University, 212005 Mogilev, Belarus

- A-VII/P2.14** MODELING OF MOLECULAR PROCESSES OF CREEP OF HIGH-ORIENTED AMORPHOUS-CRYSTALLINE POLYMER, U. Gafurov, Institute of Nuclear Physics, Ulugbek, Tashkent 702132, Uzbekistan
- A-VII/P2.15** ELECTRICAL DOMAINS IN THE SILICON CARBIDE  $n^+ - n^- - n^+$  DIODE AND IN THE STATIC INDUCTION TRANSISTOR, V.I. Sankin, P.P. Shkrebiy, A.A. Lepneva, A.F. Ioffe Physicotechnical Institute, 194021 St. Petersburg, Russia
- A-VII/P2.16** SOME THEORETICAL FOUNDATIONS OF COMPUTATIONAL MATERIALS SCIENCE ACROSS TIME AND LENGTH SCALES, S.A. Beznosyuk, A.V. Kolesnikov, D.A. Mezentsev, Altai State University, Dimitrov Street 66, 656099 Barnaul, Russia, M.S. Zhukovsky, T.M. Zhukovsky, Altai Technical State University, Lenina Street, 46, 656099 Barnaul, Russia
- A-VII/P2.17** TRANSPORT PROPERTIES OF AL-SI SOLID SOLUTIONS: THEORY, E.I. Isaev, D.V. Livanov, S.I. Manokhin, Moscow State Institute of Steel and Alloys - Technological University, Moscow, Russia, S.I. Simak, Chalmers/Gothenburg University, Gothenburg, Sweden
- A-VII/P2.18** EXPERIMENTAL INVESTIGATION AND MONTE CARLO SIMULATION OF ORDERING KINETICS IN FePdLiO, L. Messad, A. Kerrache, H. Bouzar, M. Zemirli, Institut des Sciences Exactes, Université de Tizi-Ouzou, Tizi-Ouzou, Algérie, V. Pierron-Bohnes and M.C. Cadeville, IPCMS-GEMM, 23 rue du Loess, 67037 Strasbourg, France

**Friday, June 8, 2001**  
Vendredi 8 juin 2001

**Morning**  
Matin

**Session VIII: Devices**

- A-VIII.1** 9:00 -Invited- ATOMISTIC SIMULATIONS AND THE REQUIREMENTS OF PROCESS SIMULATORS FOR NOVEL SEMICONDUCTOR DEVICES, **A. La Magna**<sup>(a)</sup>, S. Coffa<sup>(a)</sup>, S. Libertino<sup>(a)</sup>, M. Strobel<sup>(a,b)</sup>, L. Colombo<sup>(c)</sup>, <sup>(a)</sup>CNR-IMETEM Stradale Primosole 50, 95121 Catania, Italy, <sup>(b)</sup>MIRIAM, University of Milan, Milan, Italy, <sup>(c)</sup>INFM and Dipartimento di Fisica, Università di Cagliari, Cittadella Universitaria, 09042 Monserrato (Ca), Italy
- A-VIII.2** 9:30 DO ARSENIC INTERSTITIALS REALLY EXIST IN As-RICH GaAs LAYERS?, **T.E.M. Staab**, R.M. Nieminen, Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, 02015 HUT, Finland, M. Luysberg, Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany, G. Zollo, Dipartimento di Energetica e I.N.F.M., Università "La Sapienza" di Roma, via A. Scarpa 14-16, 00161 Roma, Italy, J. Gebauer, Fachbereich Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany, M. Haugk, Th. Frauenheim, University GH Paderborn, Department of Physics, Theoretical Physics, 33098 Paderborn, Germany
- A-VIII.3** 9:45 MONTE CARLO SIMULATIONS OF THE STRUCTURE, STRESS FIELD AND COMPOSITION OF Ge QUANTUM DOTS ON Si(001), **Ph. Sonnet**<sup>(a)</sup>, P.C. Kelires<sup>(a,b)</sup>, <sup>(a)</sup>Foundation for Research and Technology-Hellas (FORTH), P.O. Box 1527, 711 10 Heraclion, Crete, Greece; <sup>(b)</sup>Physics Department, University of Crete, P.O. Box 2208, 710 03 Heraclion, Crete, Greece
- A-VIII.4** 10:00 MICROSCOPIC MECHANISM OF THERMAL SILICON OXIDE GROWTH, **M. Uematsu**, H. Kageshima and K. Shiraishi, NTT Basic Research Laboratories, 3-1 Morinosato-Wakamiya, Atsugi-shi 243- 0198, Japan
- A-VIII.5** 10:15 USE OF EFFECTIVE POTENTIALS BASED ON THE ELECTRONEGATIVITY EQUALIZATION FOR THE STUDY OF INTERFACES, **S. Carniato**, N. Capron and G. Boureau, Laboratoire de chimie physique 11, rue Pierre et Marie Curie 75231 Paris Cedex 05, France
- 10:30 **BREAK**
- A-VIII.6** 11:00 COMPUTATIONAL STUDY OF MOLYBDENUM/OXIDE INTERFACES, **C.B. Geller**, Bettis Atomic Power Laboratory, West Mifflin, PA, USA, J. Sticht and E. Wimmer, Materials Design, Oceanside CA, USA and Le Mans, France
- A-VIII.7** 11:15 TITANIUM DIOXIDE AS AN ELECTRODE MATERIAL, **M.V. Koudriachova**<sup>(a)</sup>, N.M. Harrison<sup>(b)</sup>, S.W. de Leeuw<sup>(a)</sup>, <sup>(a)</sup>Delft University of Technology, Delft, Netherlands, <sup>(b)</sup>Imperial College of Science and Technology, London, UK
- A-VIII.8** 11:30 MULTI-LEVEL MODELLING STUDY OF INITIAL OXYDATION OF Si(100) UNDER WATER EXPOSURE PROVIDING MECHANISMS AND KINETICS, **A. Esteve**, M. Djafari-Rouhani, Laboratoire d'Analyse et d'Architecture des Systèmes, 7 Av. du Colonel Roche, 31077 Toulouse, France, Y. Chabal, K. Raghavachari, M. Weldon, Lucent Technologies Bell Laboratories, 600 Mountain Avenue, NJ 07974 Murray Hill, USA

- A-VIII.9** 11:45 COMBINING MONTE CARLO SIMULATIONS AND AB-INITIO CALCULATIONS IN UNDERSTANDING OF WET CHEMICAL ETCHING OF Si, M.A. Gosalvez, A.S. Foster and R.M. Nieminen, Laboratory of Physics, Helsinki University of Technology, P.O.Box 1100, 02015 HUT, Finland
- A-VIII.10** 12:00 AN ATOMISTIC MODEL OF SILICON DIOXIDE WEAR-OUT, G. Bersuker, A. Korkin\*, and H.R. Huff, International SEMATECH, 2706 Montopolis Drive, Austin Texas 78741-6499, USA; \*Semiconductor Products Sector, Motorola, Mesa AZ 85202, USA
- 12:15 **LUNCH**

**Friday, June 8, 2001**  
Vendredi 8 juin 2001

**Afternoon**  
Après-midi

**Session IX: Electronic Structure**

- A-IX.1** 14:00 CERIUM OXIDE AS OXYGEN STORAGE MATERIAL: A FIRST PRINCIPLES STUDY, S.I. Simak, N.V. Skorodumova and B.I. Lundqvist, Chalmers/Gothenburg University, Gothenburg, Sweden, I.A. Abrikosov, R. Ahuja and B. Johansson, Uppsala University, Uppsala, Sweden
- A-IX.2** 14:15 NON-EMPIRICAL STUDY OF PHASE COMPETITION IN A2-B2 MIXTURE IN FE-AL ALLOY, S. Dorfman, Dept Phys, Technion, 32000 Haifa, Israel; D. Fuks and V. Liubich, Mater Engin Dept, Ben-Gurion University of the Negev, Beer-Sheva, Israel
- A-IX.3** 14:30 POTENTIALITY OF DFT BASED CALCULATIONAL METHODS IN PREDICTING DEEP-ELECTRON SPECTROSCOPIC PROPERTIES OF CNX COMPOUNDS, M. Mattesini<sup>(a)</sup>, N. Borglund<sup>(b)</sup>, S. F. Matar<sup>(a)</sup> and S. Csillag<sup>(b)</sup>, <sup>(a)</sup>Institut de Chimie de la Matière Condensée de Bordeaux, I.C.M.C.B-CNRS, 87, Avenue du Dr. Albert Schweitzer, 33608 Pessac Cedex, France, <sup>(b)</sup>Department of Physics, Stockholm University, P.O. Box 6730, 113 85 Stockholm, Sweden.
- A-IX.4** 14:45 TRANSPORT PROPERTIES OF LIQUID MANGANESE CALCULATED FROM FIRST-PRINCIPLES MUFFIN-TIN POTENTIALS, H. Zrouri, Laboratoire de Physique du Solide, Faculté des Sciences, Université Mohammed I, Oujda, Maroc, D. Fristot and J. Hugel, IPC-LPLI, Université de Metz, 1 bd Arago, 57078 Metz Cedex 3, France
- A-IX.5** 15:00 A TIGHT BINDING INVESTIGATION OF THE ELECTRONIC STRUCTURE OF ZINC-BLENDE AND WURTZITE III-V NITRIDE SEMICONDUCTORS, B. Bouhafs<sup>(a)</sup>, F. Litimein<sup>(a)</sup>, J. Chen<sup>(b)</sup>, P. Ruterana<sup>(b)</sup> and G. Nouet<sup>(b)</sup>, <sup>(a)</sup>Computational Materials Science Laboratory, Université de Sidi-Bel-Abbès, Algérie, <sup>(b)</sup>ESCTM-CRISMAT, ISMRA 6 Bd Maréchal Juin, 14050 Caen Cedex, France
- A-IX.6** 15:15 TIGHT-BINDING MODEL FOR CALCULATION OF ELECTRONIC STRUCTURE OF INTERCALATED CARBON NANOTUBES, Yu.I. Prylutskyi<sup>(a)</sup>, O.V. Ogloblya<sup>(b)</sup>, P. Scharff<sup>(c)</sup> and P. Eklund<sup>(d)</sup>, Department of <sup>(a)</sup>Biophysics and <sup>(b)</sup>Physics, Kyiv National Shevchenko University, Volodymyrska Str. 64, 01033 Kyiv, Ukraine; <sup>(c)</sup>Institute of Physics, TU Ilmenau, 98684 Ilmenau, Germany; <sup>(d)</sup>Department of Physics, Penn State University, University Park, PA 16802-6300, USA