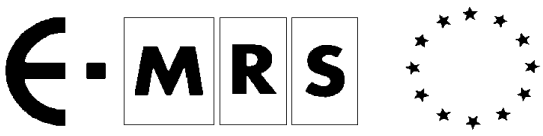

Strasbourg (France)

E-MRS Spring Meeting 2004
May 24-28, 2004

SYMPOSIUM H

Atomic scale materials design; modelling and characterization

Symposium Organizers:

Alain Estève, CNRS – LAAS, Toulouse, France

Jim Greer, University College, Cork, Ireland

Mehdi Djafari Rouhani, University of Toulouse, France

Anatoli Korkin, NANO & GIGA SOLUTIONS, Gilbert AZ, USA

Papers will be published in Computational Materials Science

E-MRS 2004 SPRING MEETING

SYMPOSIUM H

Tuesday, May 25, 2004 Morning

Session I: Polymer materials
Session chair: M. Baskes

H-I.01 09:00 -Invited- VAN DER WAALS DENSITY FUNCTIONAL THEORY CALCULATIONS OF POLYMER INTERACTIONS
Jesper Kleis and Elsebeth Schröder, Department of Applied Physics, Chalmers University of Technology and Göteborg University, 41296 Gothenburg, Sweden

H-I.02 09:30 MODELING CURRENT TRANSPORT IN ORGANIC LIGHT-EMITTING DEVICES (OLEDs)
H.L. Kwok, Centre for Advanced Materials and Related Technologies, University of Victoria, Victoria V8W 3P6, Canada

H-I.03 09:45 STABILITY IN POLYSILANES FOR LIGHT EMITTING DIODES
Asha Sharma(a), U. Lourderaj(b), Deepak(a), N. Sathyamurthy(b) and Monica Katiyar(a), (a)Dept. of Materials & Metallurgical Engg. & Samtel Centre for Display Technology, Indian Institute of Technology, Kanpur, India, (b)Dept. of Chemistry, Indian Institute of Technology, Kanpur, India

H-I.04 10:00 DENSITY FUNCTIONAL TIGHT BINDING SIMULATION OF ACETONITRILE UNDER HIGH PRESSURE
Sylvain Beaucamp and Didier Mathieu, Commissariat à l'Energie Atomique, Centre du Ripault, BP16, 37260 Monts, France and Viatcheslav Agafonov, Laboratoire de Chimie Physique, EA PIMIR 2098, Faculté de Pharmacie, 31 Avenue Monge, 37200 Tours, France

10:15 **BREAK**

Session II: Oxide materials I
Session chair: A. Estève

H-II.01 10:45 -Invited- CHARACTERISATION OF OXIDE DISPERSION-STRENGTHENED STEEL BY EXTENDED X-RAY ABSORPTION SPECTROSCOPY
C. Degueldre(a), S. Conradson(b) and W. Hoffelner(a), (a)Laboratory for Material Behaviour, Paul Scherrer Institute, 5232 Villigen, Switzerland, (b)Los Alamos National Laboratory, Los Alamos NM 87545, USA

H-II.02 11:15 -Invited- MULTIMILLION ATOM MOLECULAR DYNAMICS SIMULATIONS OF NANOSTRUCTURES ON PARALLEL COMPUTERS
P. Vashishta, University of Southern California, USA

H-II.03 11:45 -Invited- MONTE CARLO SIMULATIONS OF SILICON NANOCRYSTALS IN AMORPHOUS SILICON DIOXIDE
G. Hadjisavvas and **P.C. Kelires**, Physics Department, University of Crete, P.O. Box 2208, 710 03 Heraclion, Crete, Greece

H-II.04 12:15 A DENSITY FUNCTIONAL THEORY STUDY OF THE OXIDATION OF THE Si-RICH SiC SURFACE
E. Wachowicz(a,b), R. Rurali(c,d), P. Ordejon(c) and P. Hyldgaard(a), (a)Department of Applied Physics, Chalmers University of Technology, 41296 Göteborg, Sweden, (b)Institute of Experimental Physics, University of Wroclaw, Pl. Maxa Borna 9, 50294 Wroclaw, Poland, (c)Institut de Ciencia de Materials de Barcelona (ICMAB--CSIC), Campus de Bellaterra, 08193 Barcelona, Spain, (d)Laboratoire Collisions, Agrégats, Réactivité, UMR5589, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse cedex, France

H-II.05 12:30 LAYERED SURFACE-OXIDE STRUCTURES ON Mg(0001)
Elsebeth Schroder(a) and Adam Kiejna(b), (a)Department of Applied Physics, Chalmers University of Technology and Goteborg University, 41296 Gothenburg, Sweden, (b)Institute of Experimental Physics, University of Wroclaw, Plac M. Borna 9, 50-204 Wroclaw, Poland

12:45 **LUNCH**

Tuesday, May 25, 2004 Afternoon

Session III: Metals and inter-metallic materials
Session chair: P. Vashishta

H-III.01 14:00 -Invited- USING ATOMISTIC MODELING FOR MATERIALS DESIGN
M.I. Baskes, Los Alamos National Laboratory, USA

H-III.02 14:30 POLARIZATION BEHAVIOUR IN SYSTEMS WITH COMPETING FERROELECTRIC/ANTIFERROELECTRIC INTERACTIONS
J. Milhazes, A. Cadilhe and S. Lanceros-Méndez, Centro de Física da Universidade do Minho, 4710-057 Braga, Portugal

H-III.03 14:45 THE RESEARCH OF THE MECHANISM OF NON-VACATIONAL DISORDERING IN A TWO-DIMENSIONAL ALLOY OF Ni3Al INTERMETALLIDE
M.D. Starostenkov, M.B. Kondratenko, N.B. Cholodova, G.M., Poletaev, Altai State Technical University, Department of General Physics, Barnaul, Lenin st. 46, Barnaul 656038, Russia

H-III.04 15:00 COMPUTER SIMULATION STUDY OF DISLOCATION DYNAMICS IN MOLYBDENUM
Y.L. Liu and C.H Woo, Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong SAR, China

H-III.05 15:15 MULTI-SCALE MODELING OF MIGRATION AND STABILITY OF ELEMENTARY DEFECTS IN ALPHA-IRON
J. Dalla Torre, C.C. Fu, F. Willaime, J.-L. Bocquet, A. Barbu, Service de Recherches de Métallurgie Physique, CEA/Saclay, France

H-III.06 15:30 FP-LAPW INVESTIGATIONS OF ELECTRONIC STRUCTURE OF TaN AND TaC COMPOUNDS
M. Sahnoun(a), C. Daul(a), C. Demangeat(b), J.C. Parlebas(b) and M. Driz(c), (a)Département de Chimie, Université de Fribourg, Pérolles, 1700 Fribourg, Switzerland, (b)IPCMS-GEMM, UMR 7504 CNRS, 23, rue du Loess, 67034 Strasbourg Cedex 2, France, (c)Laboratoire de Sciences des Matériaux, Université Djillali Liabes - Sidi Bel Abbes, Algeria

15:45 **BREAK**

Session IV: Deposition techniques and growth
Session chair: P.C. Kelires

H-IV.01 16:15 -Invited- VAPOR DEPOSITION OF THIN METALLIC FILMS: ATOMISTIC MONTE CARLO SIMULATIONS
J. Dalla Torre, Service de Recherches de Métallurgie Physique, CEA/Saclay, France

H-IV.02 16:45 -Invited- SEEDING GROWTH OF SURFACE-ALIGNED NANOSTRUCTURES BY SURFACE ASSEMBLY OF ATOM-SCALE METALLIC WIRES
Per Hyldgaard and Bengt I. Lundqvist, Department of Applied Physics, Chalmers University of Technology, 41296 Gothenburg, Sweden

H-IV.03 17:15 SELF-ORGANIZATION IN A MODEL OF STRAINED EPITAXY
Vasyl Tokar(a,b) and Hugues Dreyssé(a), (a)Institut de Physique et Chimie des Matériaux de Strasbourg, 23 rue du Loess, 67037 Strasbourg, France, (b)Institut of Magnetism, National Academy of Sciences 36-b Vernadsky str, 03142 Kiev-142, Ukraine

H-IV.04 17:30 MODELLING OF LAYER EPITAXIAL GROWTH: SURFACE MORPHOLOGY AND GROWTH MODE TRANSITIONS
Vladimir I. Trofimov, Ilya V. Trofimov, Institute of Radioengineering & Electronics of RAS, 11/7 Mokhovaya Street, 125009 Moscow, Russia and Jong-Il Kim, School of Information Technology and Engineering Korea University of Technology and Education, Chung Nam-Do, 330-708 Seoul, Korea

H-IV.05 17:45 MORPHOLOGICAL INSTABILITIES AND CRITICAL THICKNESS FOR DISLOCATION GENERATION IN EPITAXIAL THIN FILMS
Biao Wang and C.H. Woo, Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong SAR, China

H-IV.06 18:00 GROWTH OF THE THREE-DIMENSIONAL SiC CLUSTERS ON Si MODELLED BY KMC
J. Pezoldt, FG Nanotechnologie, Zentrum für Mikro- und Nanotechnologien, TU Ilmenau, Postfach 100565, 98684 Ilmenau, Germany, A.A. Schmidt, V.S.Kharlamov, K.L. Safonov and Yu.V. Trushin A.F. Ioffe Physico-Technical Institute, Polytekhnicheskaya 26, 194021 St. Petersburg, Russia, E.E.Zhurkin, St.Petersburg State Polytechnic University, Polytekhnicheskaya 29, 195251 St. Petersburg, Russia

Wednesday, May 26, 2004 Afternoon

Session V: Nanostructure properties
Session chair: M. Djafari Rouhani

H-V.01 14:00 -Invited- ATOMIC-SCALE STM EXPERIMENTS ON SEMICONDUCTOR SURFACES/ TOWARDS MOLECULAR NANOMACHINES
Prof. Dujardin, Laboratoire de Photophysique Moléculaire, Orsay, France

H-V.02 14:30 STRUCTURAL DEPENDENCE OF OPTICAL PROPERTY OF SINGLE-WALLED BORON NITRIDE NANOTUBES
R.Q. Zhang and M.F. Ng, Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, China

H-V.03 14:45 SELF-ORGANIZING PROCESSES IN CRYSTAL LATTICES AND FORMATION OF STRUCTURES OF NANOMETER DIMENSIONS
I.V. Tereshko, V.V. Glushchenko, A.M. Tereshko, R.V. Petrov and V.V. Abidzina, Belarusian - Russian University, Prospect Mira 43, 212005 Mogilev, Belarus

H-V.04 15:00 L10- ORDERING KINETICS IN FePt NANO-LAYERS: MONTE CARLO SIMULATION
M. Kozlowski, R. Kozubski, Institute of Physics, Jagellonian University, Reymonta 4, 30-059 Krakow, Poland, V. Pierron-Bohnes, Institut de Physique et Chimie des Matériaux de Strasbourg, 23, rue du Loess, BP43, 67034 Strasbourg CEDEX 2, France

H-V.05 15:15 NANOSCALE EFFECTS ON THE NANOMECHANICAL PROPERTIES OF MULTIFUNCTIONAL MATERIALS
C. Charitidis, S. Logothetidis, Laboratory for Thin Films, Nanosystems and Nanometrology, Department of Physics, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

H-V.06 15:30 MODELING THE OPTICAL PROPERTIES OF SI-CAPPED GERMANIUM QUANTUM DOTS
N. Skoulidis, H. Polatoglou, Department of Physics, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

H-V.07 15:45 MODELLING OF A SELFORGANIZATION PROCESS LEADING TO PERIODIC ARRAYS OF NANOMETRIC AMORPHOUS PRECIPITATES BY ION IRRADIATION
F. Zirkelbach, M. Häberlen, J.K.N. Lindner and B. Stritzker, Universität Augsburg, Universitätsstrasse 1, 86135 Augsburg, Germany

16:00 **BREAK**

Session VI: Quantum investigation of complex systems
Session chair: J. Greer

H-VI.01 16:30 -Invited- THE STEADY-STATE OF HETEROGENEOUS CATALYSIS STUDIED BY FIRST-PRINCIPLES STATISTICAL MECHANICS
Prof. Reuter, Fritz-Haber-Institut, Germany

H-VI.02 17:00 -Invited- NANOCATALYSIS WITH ALUMINAS
S.T. Pantelides, S. Rashkeev, S. Wang. K. Sohlberg, M. Glasoff, A. Borisevitch, S.J. Pennycook, Vanderbilt University, Nashville, TN, USA, and Oak Ridge National, Laboratory, Oak Ridge TN, USA

H-VI.03 17:30 -Invited- AB INITIO CALCULATIONS OF ELECTRONIC EXCITATIONS/ CHALLENGES AND RECENT PROGRESS
Prof. Reining, Laboratoire des Solides Irradiés, Polytechnique, France

H-VI.041 18:00 QUANTUM MECHANICAL CALCULATION OF SOLID STATE EQUILIBRIUM RUTHENIUM AND RHODIUM RUTILE VS CORUNDUM PHASES
M.H. Grillo, Accelrys GMBH, Germany

H-VI.05 18:15 THEORETICAL INVESTIGATION ON THE GRAFTING OF CHAIN ORGANO-SILANES ON SILICA SURFACES
A. Dkhissi, L. Jeloaica, A. Estève and M. Djafari Rouhani, LAAS-CNRS, France

Thursday, May 27, 2004 Morning

Session VII: Surfaces
Session chair: J. Gavartin

H-VII.01 08:30 -Invited- AN AB INITIO STUDY OF TITANIUM-TETRA-ISO-PROPOXIDE (TTIP) ABSORPTION MECHANISM ON Si (100) SURFACE
A. Palma, Istituto per lo Studio dei Materiali Nanostrutturati (CNR-ISMN), Via Salaria Km 29.3, 00016 Monterotondo Scalo (RM), Italy and A. Alavi, Chemistry Department, University of Cambridge, Lansfield Road, Cambridge, U.K.

H-VII.02 09:00 INVESTIGATION OF SPUTTERING AND OXYGEN DESORPTION PROCESSES BY BINARY COLLISION APPROXIMATION METHOD
A.A. Dzhurakhalov and S.E. Rahmatov, Arifov Institute of Electronics, F.Khodjaev Str.33, 700125 Tashkent, Uzbekistan

H-VII.03 09:15 THE PECULIARITIES OF THE INTERACTION OF DIVACANCIES WITH INTERSTITIAL BOUNDARIES IN TWO-DIMENSIONAL COMPOSITES OF NI3AL-AL AND NI3AL-NI SYSTEMS
M.D. Starostenkov, E.A. Dudnik, General Physics Department, Altai State Technical University, 46 Lenin st, 656038 Barnaul, Russia and I.A. Demina, G.V. Popova, East-Kazakhstan State University, 19 Serikbaeva st, 492010 Ust-Kamenogorsk, Kazakhstan

H-VII.04 09:30 -Invited- STABILITY, ELECTRONIC AND STRUCTURAL PROPERTIES OF DEFECTED ZNSE/GAAS(001) HETEROSTRUCTURES
A. Stroppa, M. Peressi Universita' degli Studi di Trieste, 34100 Trieste, Italy and INFM-DEMOCRITOS Simulation Center, Trieste, Italy

H-VII.05 09:45 MAINTAINING HALF METALLICITY AT NiMnSb/III-V SEMICONDUCTOR HETEROJUNCTIONS: THE ROLE OF SEMICONDUCTOR SUBSTRATE AND LOCAL INTERFACE TERMINATION A. Debernardi(a), M. Peressi(a,b) and A. Baldereschi(a,b,c), (a)Istituto Nazionale di Fisica della Materia (INFM), DEMOCRITOS Research Unit of Trieste, via Beirut 4/2, 34014 Trieste, Italy, (b)Department of Theoretical Physics, University of Trieste, Strada Costiera 11, 34014 Trieste, Italy, (c)Ecole Politechnique Federal de Lausanne (EPFL), 1015 Lausanne, Switzerland

H-VII.06 10:00 TIGHT BINDING MODELLING OF BAND OFFSETS IN NANOSCALE HETEROSTRUCTURES H. Hakan Gürel, Özden Akonco and Hilmi Ünlü, Department of Physics & Informatics Institute, Istanbul Technical University, Maslak Istanbul 80626, Turkey

10:15 **BREAK**

10:45-12:45 POSTER SESSION

H/P.01 COEXISTENCE OF HIGH TEMPERATURE SUPERCONDUCTIVITY AND ANTIFERROMAGNETISM
Krzysztof Kucab, Grzegorz Górski, Stanislaw Topolewicz and Jerzy Mizia Institute of Physics, University of Rzeszów, Poland

H/P.02 MODEL BASED OPTIMIZATION OF SOME GROWTH PROCESS PARAMETERS OF A Nd:YAG CYLINDRICAL BAR GROWN BY EDGE -DEFINED FIM-FED GROWTH (E.F.G.) METHOD
L. Braescu, Department of Mathematics, Polytechnical University of Timisoara, P-ta Regina Maria No. 1, Timisoara 300004, Romania, A.M. Balint, Department of Physics, West University of Timisoara, Blv. V. Parvan No.4, Timisoara 300223, Romania, St. Balint, Department of Mathematics, West University of Timisoara, Blv. V. Parvan, No.4, Timisoara 300223, Romania

H/P.03 MODEL BASED PREDICTION OF THE EFFECTS OF THE OSCILLATIONS OF THE PRESSURE IN THE FURNACE IN THE CASE OF AN EDGE-DEFINED FIM-FED GROWTH SYSTEM
L. Braescu, Department of Mathematics, Polytechnical University of Timisoara, P-ta Regina Maria No. 1, Timisoara 300004, Romania, A.M. Balint, Department of Physics, West University of Timisoara, Blv. V. Parvan No.4, Timisoara 300223, Romania, St. Balint Department of Mathematics, West University of Timisoara, Blv. V. Parvan No.4, Timisoara 300223, Romania

H/P.04 A MODEL BASED CONTROL PROCEDURE FOR OF THE SHAPE OF A Nd:YAG CYLINDRICAL BAR GROWN BY EDGE-DEFINED FILM-FED GROWTH (E.F.G.) METHOD WHEN THE PRESSURE IN THE FURNACE OSCILLATES
L. Braescu, Department of Mathematics, Polytechnical University of Timisoara, P-ta Regina Maria No. 1, Timisoara 300004, Romania, A.M. Balint, Department of Physics, West University of Timisoara, Blv. V. Parvan No.4, Timisoara 300223, Romania, St. Balint, Department of Mathematics, West University of Timisoara, Blv. V. Parvan No.4, Timisoara 300223, Romania

H/P.05 EFFECTS OF METALLIC CONTACTS ON SILICON NANOSTRUCTURES STUDIED QUANTUM MECHANICALLY
C. Summonte and A.M. Mazzone, C.N.R.-Istituto IMM, Sezione di Bologna, Via Gobetti 101, 40129 Bologna, Italy

H/P.06 MOLECULAR DYNAMICS SIMULATIONS OF ATOMIC-SCALE SLIDING FRICTION OF a-, nc-SiC AND c-C SURFACES
V.I. Ivashchenko, P.E.A. Turchi(b), V.I. Shevchenko(a), L.A. Ivashchenko(a) and O.K. Porada(a), (a)Institute of Problems of Material Science, NAS of Ukraine, Krzhyzhanovsky Str. 3, 03680 Kyiv-142, Ukraine, (b)Lawrence Livermore National Laboratory (L-353), P.O. Box 808, Livermore CA 94551, USA

H/P.07 MOLECULAR DYNAMICS SIMULATIONS OF THE ATOM-BY-ATOM DEPOSITION OF a-SiC FILMS
V.I. Ivashchenko(a), P.E.A. Turchi(b), V.I. Shevchenko(a), L.A. Ivashchenko(a), O.K. Porada(a), and G.V. Rusakov(a), (a)Institute of Problems of Material Science, NAS of Ukraine, Krzhyzhanovsky Str. 3, 03680 Kyiv-142, Ukraine, (b)Lawrence Livermore National Laboratory (L-353), P.O. Box 808, Livermore, CA 94551, USA

H/P.08 CURRENT TRANSPORT IN A SILICON NANOWIRE ENDED BY ALUMINUM ATOMS
A.M. Mazzone and V. Morandi, C.N.R.-Istituto IMM, Sezione di Bologna, Via Gobetti 101, 40129 Bologna, Italy

H/P.09 THE LOCAL INELASTIC ELECTRON -POLAR OPTICAL PHONON INTERACTION IN MERCURY TELLURIDE
O.P. Malyk, Lviv Polytechnic National University, Semiconductor Electronics Department, Bandera Street 12, 79013 Lviv-13, Ukraine

H/P.10 THE EXACT SOLUTION OF A STATIONARY BOLTZMANN EQUATION FOR THE SEMICONDUCTOR WITH ISOTROPIC DISPERSION LAW
O.P. Malyk, Lviv Polytechnic National University, Semiconductor Electronics Department, Bandera Street 12, 79013 Lviv-13, Ukraine

H/P.11 THE ADSORPTION OF ETHYLENE ON THE Si(001)(2x1) SURFACE BY COAXIAL IMPACT COLLISION ION SCATTERING SPECTROSCOPY
J.H. Seo(a), J.Y. Park(a), J.Y. Kim(a), S.S. Kim(b), C.H. Chae(c), D.S. Choi(d), C.N. Whang(a), (a)Atomic-scale Surface Science Research Center and Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea, (b)Department of Physics, Mokwon University, Taejon 301-729, Korea, (c)Material Science and Engineering Division, Korea Institute of Science and Technology, Seoul 130-650, Korea, (d)Department of Physics, Kangwon National University, Chuncheon 200-701, Korea

H/P.12 DIFFUSION-LIMITED REGIMES IN PERCOLATIVE TO COMPACT SUBSTRATES
N.J.A.P. Gonçalves(a,c), J.A.M.S. Duarte(b) and A. Cadilhe(a), (a)Centro de Física da Universidade do Minho, 4710-057 Braga, Portugal, (b)Centro de Matemática Aplicada da Universidade do Porto, 4169-007 Porto, Portugal, (c)Departamento de Física, Universidade de Trás-os-Montes e Alto Douro, 5000-911 Vila Real, Portugal

H/P.13 MONTE CARLO GROWTH AND IN SITU CHARACTERISATION FOR AlxGa1-xAs HETEROEPITAXY
N. Fazouan(a), M. Djafari. Rouhani(b,c), D. Esteve(c), (a)Laboratoire de Physique des Matériaux, Faculté des Sciences et Techniques, BP 523, 23000 Béni Mellal, Maroc, (b)Laboratoire de Physique des Solides, Université Paul Sabatier, 118 Route de Narbonne, 31062 Toulouse Cedex, France, (c)Laboratoire d'Analyse et d'Architecture des Systèmes, 7 avenue du Colonel Roche, 31077 Toulouse Cedex, France

H/P.14 NANO-SCALE DECOMPOSITION IN DESCONTINUOUSLY TRANSFORMED Fe-Ni-Cr-N ALLOYS UPON AGING
V. Delvaux and G. Solórzano, Departamento de Ciência dos Materiais e Metalurgia - Pontifícia Universidade Católica do Rio de Janeiro, RJ, Brazil

H/P.15 Cu-ALKALI ION EXCHANGE IN GLASS: A MODEL FOR THE COPPER DIFFUSION BASED ON XAFS EXPERIMENTS
F. Gonella, INFM, Physical Chemistry Dept., University of Venezia, Dorsoduro 2137, 30123 Venezia, Italy, A. Quaranta, INFM, Materials Engineering Dept., University of Trento, via Mesiano 77, 38050 Povo, Trento, Italy, E. Cattaruzza, S. Padovani, C. Sada, INFM, Physics Dept., University of Padova, via Marzolo 8, 35131 Padova, Italy, F. D'Acapito, C. Maurizio, INFM, GILDA CRG c/o ESRF, BP 200, 38043 Grenoble, France

H/P.16 ERBIUM AND SILVER LOCAL ENVIRONMENT IN CO-DOPED GLASSES FOR OPTICAL AMPLIFICATION
S. Padovani, E. Cattaruzza, F. Enrichi, G. Mattei, P. Mazzoldi, C. Sada, E. Trave, INFM, Physics Dept., University of Padova, via Marzolo 8, 35131 Padova, Italy, F. Gonella, INFM, Physical Chemistry Dept., University of Venezia, Dorsoduro 2137, 30123 Venezia, Italy, F. D'Acapito, C. Maurizio, INFM, GILDA CRG c/o ESRF, BP 200, 38043 Grenoble, France, M. Guglielmi, A. Martucci, Mechanical Engineering Dept., University of Padova, via Marzolo 9, 35131 Padova, Italy

H/P.17 EXTENDED MOLECULAR DYNAMICS SIMULATIONS OF INTERFACES AND DEFECTS: ELASTIC FLEXIBLE BOUNDARY CONDITIONS
A.Yu. Belov, Technical University of Dresden, Hallwachsstr. 3, 01069 Dresden, Germany and K. Scheerschmidt, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

H/P.18 GENETIC ALGORITHM APPROACH FOR NANOSCALE CONDUCTING WIRES
Hiroshi Mizuseki, Nobuaki Igarashi, Rodion V. Belosludov, Amir A. Farajian, and Yoshiyuki Kawazoe, Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

H/P.19 MONTE-CARLO SIMULATION OF GIANT MAGNETORESISTANCE AND PHASE SEPARATION IN A RANDOM-FIELD MAGENETIC POLARON MODEL
Sh. Dong, H. Yu, K.-F Wang, X.Y. Yao, and J.–M. Liu, Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China

H/P.20 MONTE-CARLO SIMULATION ON THE DIPOLE ALIGNMENT IN FERROELECTRIC SQUARE LATTICE
X. Wang and J.–M. Liu, Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China

H/P.21 BUCKY SHUTTEL MEMORY SYSTEM BASED ON BORON-NITRDIE NANOPEAPOD
Won Young Choi, Jeong Won Kang and Ho Jung Hwang, Chung-Ang University, Seoul, Korea

H/P.22 QUANTITATIVE CHARACTERIZATION OF THE MESOSCOPIC SURFACE ROUGHNESS IN A GROWING ISLAND FILM
Vladimir I. Trofimov, Ilya V. Trofimov, Institute of Radioengineering & Electronics of RAS, 11/7 Mokhovaya Street, 125009 Moscow, Russia and Jong-Il Kim, School of Information Technology and Engineering Korea University of Technology and Education, Chung Nam-Do, 330-708 Seoul, Korea

H/P.23 ELECTROMAGNETIC CHARACTERISTICS OF YBCO CERAMICS SUPERCONDUCTOR
Sang Heon Lee, Department of Electronics Information and Communication Engineering, Sun Moon University, Asan, Chung Nam, South Korea

H/P.24 ELECTROMAGNETIC PROPERTIES OF BPSCCO CERAMICS
Sang Heon Lee, Department of Electronics Information and Communication Engineering, Sun Moon University, Asan, Chung Nam, South Korea

H/P.25 MEASUREMENT OF ATTRACTION FORCE BETWEEN AFM TIP AND SURFACE OF DIELECTRIC THIN FILMS WITH DC-BIAS
Y.F. Zhu, C.H. Xu, B. Wang and C.H. Woo, Department of Mechanical Engineering, The Hongkong Polytechnic University Hung hom, Kowloon, Hongkong, China

H/P.26 AB INITIO SIMULATIONS ON AgCl(111) SURFACE AND AgCl(111)/a-Al2O3(0001) INTERFACE.
Yuri F. Zhukovskii(a), Eugene A. Kotomin(a,b), Yuri Mastrikov(b) and Joachim Maier(b), (a)Institute of Solid State Physics, University of Latvia, Kengaraga 8, Riga 1063, Latvia, (b)Max-Planck-Institut für Festkörperforschung, Heisenbergstr.1, Stuttgart 70569, Germany

H/P.27 KINETIC MODEL FOR PRODUCTION AND GROWTH OF DUST PARTICLES IN THE PLASMAS OF ELECTRONEGATIVE GASES
B.F. Gordiets*, A. Pinyol and E. Bertran, Departament de Fisica Aplicada i Optica, Universitat de Barcelona. Avinguda Diagonal 647, 08028 Barcelona, *On leave from Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia

H/P.28 INTRA-MOLECULAR PROPERTIES OF DMeOPPV STUDIED BY QUANTUM MOLECULAR DYNAMICS
Helena M.G. Correia, Marta M.D. Ramos, Departamento de Física, Universidade do Minho, Largo do Paço, 4700-320 Braga, Portugal

H/P.29 QUANTUM MODELLING OF POLY(VINYLIDENE FLUORIDE)
Helena M.G. Correia, Marta M.D. Ramos, Departamento de Física, Universidade do Minho, Largo do Paço, 4700-320 Braga, Portugal

H/P.30 ATOMISTIC MODELLING OF PROCESSES INVOLVED IN POLING OF PVDF
Marta M.D. Ramos, Helena M.G. Correia, S. Lanceros-Méndez, Departamento de Física, Universidade do Minho, Largo do Paço, 4700-320 Braga, Portugal

H/P.31 NOVEL LANTHANIDE COMPLEXES FOR VISIBLE AND IR EMISSION
F. Rizzo, A. Papagni, F. Meinardi, R. Tubino, M. Ottonelli, G.F. Musso and G. Dellepiane, Università di Milano Bicocca, Dipartimento di Scienza dei Materiali, Via Cozzi 53, 20126 Milano, Italy, Università di Genova, Dipartimento di Chimica e Chimica Industriale, Via Dodecaneso 31, 16146 Genova, Italy

H/P.32 SECOND-MOMENT INTERATOMIC POTENTIAL FOR GOLD AND ITS APPLICATION TO MOLECULAR-DYNAMICS SIMULATIONS
H. Chamati(a), N.I. Papanicolaou(b), (a)Institute of Solid State Physics, 72 Tzarigradsko Chaussee, 1784 Sofia, Bulgaria, (b)Solid State Division, Department of Physics, University of Ioannina, P.O. Box 1186, 45110 Ioannina, Greece

H/P.33 ELECTRONIC STATES ASSOCIATED WITH TILT BOUNDARY IN GaN
A. Béré, J. Chen, P. Ruterana and G. Nouet, SIFCOM/ENSICAEN, UMR CNRS 6176, 6 Bd du Maréchal Juin, 14050 Caen Cedex, France, J. Koulidiati, Departement de Physique, Université de Ouagadougou, 03 BP, 7021 Ouagadougou 03, Burkina Faso, A.T. Blumenau, Department of Physics, Universität Paderborn, 33098 Paderborn, Germany

H/P.34 NUMERICAL SIMULATION OF FILM THICKNESS DISTRIBUTION IN ELECTRON-BEAM CO-EVAPORATION
P. Aubreton, A. Bessaudou, C. Di Bin, IRCOM, CNRS, UMR 6615, équipe C2M Faculté des Sciences et Techniques 123, avenue Albert Thomas 87060 Limoges, France

H/P.35 LOCAL VIBRATIONAL MODES OF Zn-H-As DEFECTS IN GaAs, ZnSe AND ZnTe
V.J.B. Torres and J. Coutinho, Department of Physics, University of Aveiro, 3810-193 Aveiro, Portugal, P.R. Briddon, School of Natural Sciences, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU, U.K.

H/P.36 MODELIZATION OF THIN FILM GROWTH
H.M. Pinto, R.M. Ribeiro, Departamento de Física, Universidade do Minho, 4710-057 Braga, Portugal

H/P.37 ATOMIC SCALE ANALYSIS OF YBa2Cu3Oy BY LOW-ENERGY ION SCATTERING
A.A. Dzhurakhalov and I.D. Yadgarov, Arifov Institute of Electronics, F.Khodjaev Str. 33, 700125 Tashkent, Uzbekistan

H/P.38 COMPARISON OF C60 ENCAPSULATIONS INTO CARBON AND BORON-NITRIDE NANOTUBES
Jeong Won Kang, Won Young Choi, Ki Ryang Byun and Ho Jung Hwang, Computational Semiconductor Laboratory, Department of Electronic Engineering, Chung-Ang University, 221 HukSuk-Dong, DongJak-Ku, Seoul 156-756, Korea

H/P.39 MODELING OF FLUX-FLOW FOR SUPERCONDUCTING FLUX FLOW TRANSISTOR WITH NANOBRIDGE
Seokcheol Ko(a), Hyeong-Gon Kang(b), Sung-Hun Lim(c), Byoung-Sung Han(a), (a)Division of Electronics and Information Engineering, Chonbuk National University 664-14, Duckjin-Dong 1Ga, Jeonju Chonbuk 561-756, South Korea, (b)Semiconductor Physics Research Center 664-14, Chonbuk National University, Jeonju Chonbuk, 561-756, South Korea. (c)The Research Center of Industrial Technology, Engineering Research Institute, Chonbuk National University, JeonJu 561-756, South Korea

H/P.40 QUENCHING-DEPENDENT REVERSIBLE MODIFICATION OF ELECTRONIC STRUCTURE OF PROTON-IMPLANTED SILICON
S.Zh. Tokmoldin, Kh.A. Abdullin, A.T. Issova, B.N. Mukashev, A.S. Serikkanov, Institute of Physics and Technology, Ibragimov Street 11, Almaty 480082, Kazakhstan

H/P.41 ELECTRONIC EXCITATIONS IN THE Er(8-HYDROXYQUINOLINE)3 COMPLEX: A THEORETICAL STUDY USING THE SPARKLE MODEL
M. Ottonelli, G. Izzo, G.F. Musso, G. Dellepiane and F. Meinardi, INFM-INSTM-Università di Genova, Dipartimento di Chimica e Chimica Industriale, via Dodecaneso 31, 16146 Genova, Italy, Università di Milano Bicocca, Dipartimento di Scienza dei Materiali, Via Cozzi 53, 20126 Milano, Italy

H/P.42 MD SIMULATION OF LOW-ENERGY SMALL CLUSTER BOMBARDMENT OF CRYSTAL SURFACES AT GRAZING INCIDENCE
U.B. Khalilov, D.Kh. Husanova and A.A. Dzhurakhalov, Arifov Institute of Electronics, F. Khodjaev Str. 33, 700125 Tashkent, Uzbekistan

H/P.43 FORMATION OF ALUMINIDE PHASES ON Ti SUBSTRATE DURING ANNEALING AND ION IRRADIATION
S. Romankov, B. Mukashev, E. Vdovichenko, Institute of Physics and Technology, Ibragimov Street 11, Almaty 480082, Kazakhstan

H/P.44 KINETIC MODEL of THIN FILM GROWTH
B.F. Gordiets, Leave on Lebedev Physical Institute of Russian Academy of Sciences, Moscow, J.L. Andújar, C.Corbella, E.Bertran, Departament de Física Aplicada i Òptica, Universitat de Barcelona, Av.Diagonal 647, 08028 Barcelona, Spain

H/P.45 RF SPUTTERING DEPOSITION AND MAGNETIC CHARACTERISATION OF ND-FE-B THIN FILMS FOR MICROWAVE APPLICATIONS
M. Valetas, F. Cosset, A. Bessaudou and J.C. Vareille, IRCOM, C2M, 123 avenue Albert Thomas, 87060 Limoges, France

H/P.46 FIRST PRINCIPLES CALCULATION STUDY OF MULTI-SILICON DOPED FULLERENES
M. Matsubara, C. Massobrio and J.-C. Parlebas, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504 CNRS, Université Louis Pasteur, 23 rue du Loess, BP43, 67034 Strasbourg Cedex 2, France

H/P.47 STOCHASTIC SIMULATIONS OF THE SYNTHESIS OF NANOCRYSTALS IN REVERSE MICELLES
F. Mavelli(a), M.L Curri(b), M. Striccoli(b), A. Agostiano(a,b), (a)Dip. Chimica, Università degli Studi di Bari, Via Orabona 4, 70126 Bari, Italy, (b)CNR IPCF Bari Division, c/o Dip. Chimica, Università degli Studi di Bari, Via Orabona 4, 70126 Bari, Italy

H/P.48 FIRST-PRINCIPLES STUDY OF CUBIC ALxGA1-xN ALLOYS
Z. Dridi(a,b), B. Bouhafs(a,b) and P. Ruterana(a), (a)SIFCOM, UMR 6176, CNRS-ENSICAEN, 6 Boulevard Maréchal Juin, 14050 Caen Cedex, France, (b)LSMSM, Département de Physique, Faculté des Sciences, Université de Sidi-Bel-Abbès, 22000 Sidi-Bel-Abbès, Algérie

H/P.49 LOW-ENERGY P+ION CHANNELING AND IMPLANTATION INTO SI(110), SIC(110), GAP(110) AND ASGA(110)
A.M. Rasulov, Ferghana Polytechnic Institute, Ferghana Str. 86, 712022 Ferghana, Uzbekistan, A.A. Dzhurakhalov, Arifov Institute of Electronics, F. Khodjaev Str. 33, 700125 Tashkent, Uzbekistan

H/P.50 CHARACTERISATION AND DEPTH PROFILES MEASUREMENTS OF SILICON NITRIDE THIN FILMS ON SILICON AND MOLYBDENUM SUBSTRATES BY AUGER ELECTRON SPECTROSCOPY
Chakib Fakih(a), Glades Bachir Fakih(a), R.S Bes(b) and R. Berjoan(c), (a)Université Libanaise Faculté de Génie Beyrouth Liban, (b)Université Paul Sabatier, Toulouse France, (c)IMP CNRS, B.P 5, Odeillo, 66120 Font Romeu cedex, France

H/P.51 CHARACTERIZATION OF THE JAMMING STATE OF PRE-TREATED PATTERNED SURFACES BY EXTENSIVE MONTE CARLO SIMULATIONS
N. Araújo and A.M. Cadilhe, GCEP-Centro de Física da Universidade do Minho, 4710-057 Braga, Portugal, Vladimir Privman, Center for Quantum Device Technology, Clarkson University, New York, USA

H/P.52 EFFET OF TUNGSTEN 0- 8wt.% ON THE OXIDATION OF Co-Cr ALLOYS
A. Karaali(a), K. Mirouh(a), S. Hamamda(a) and P. Guiraldenq(b), (a)Département de Physique, Faculté des Sciences, Université Mentouri, Constantine, Algérie, (b)Département IFOS, Ecole Centrale de Lyon, 69131 Ecully cedex, France

H/P.53 A NANOSTRUCTURED BIOSENSOR BASED ON ENZYME IMMOBILIZATION IN LAYER-BY-LAYER FILMS
V. Zucolotto, A.P.A. Pinto, A.P.U. Araújo, O.N. Oliveira Jr., Instituto de Física de São Carlos, USP, SP, CP 369, Brazil

H/P.54 ANALYSIS OF NANO-SIZED STRUCTURES IN HYDROGENATED AMORPHOUS SILICON-CARBON THIN FILMS
D. Gracin, K. Juraic, P. Dubcek, A. Gajovic and I. Bogdanovic-Radovic, Rudjer Boskovic Institute, Zagreb, Croatia

H/P.55 QUANTITATIVE ESTIMATION OF THE ORDER-DISORDER PHASE TRANSITION TEMPERATURE OF NI3AL USING A FACE CENTERED CUBIC LATTICE MODEL WITH A RENORMALIZED POTENTIAL

Ryoji Sahara(a), Hiroshi Mizuseki(a), Kaoru Ohno(b), and Yoshiyuki Kawazoe(a), (a)Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, (b)Department of Physics, Graduate of School of Engineering, Yokohama National University, 240-8501, Yokohama, Japan

H/P.56 ATOMISTIC MODELLING OF METAL SULPHIDES

P.E. Ngoepe, S.P. Ntoahae, H.M. Sithole, Materials Modelling Centre, University of the North, Private Bag x1106, Sovenga 0727, South Africa, S.C. Parker, School of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, U.K., K.V. Wright, The Royal Institution of Great Britain, 21 Albermarle Street, London W1X 4BS, U.K.

H/P.57 TRENDS IN ATOMIC DIFFUSION ON METALLIC SURFACES

Adele Carrado, Hervé Bulou, Christine Goyhenex, Institut de Physique et Chimie des Matériaux de Strasbourg, GSI, BP 43, 67034 Strasbourg cedex 02, France

H/P.58 MOLECULAR MODELING OF DISLOCATION FORMATION AND PLASTIC DEFORMATION OF AN ORIENTED CRYSTALLINE POLYMER

U. Gafurov, Institute of Nuclear Physics, Tashkent 702132, Uzbekistan

H/P.59 ATOMIC AND ELECTRONIC STRUCTURES OF THREADING SCREW DISLOCATION IN WURTZITE GaN

Imad Belabbas, SIFCOM UMR CNRS 6176, ENSICAEN, 6 boulevard du Maréchal Juin, 14050 Caen cedex, France, Mohamed Akli Belkhir, Groupe de physique du solide, Laboratoire de physique théorique, Université A. Mira de Béjaia, Algérie, Young Hee Lee, Center for Nanotubes and Nanostructured Composites, Institute of Basic Science, Department of Physics Sungkyunkwan University, Suwon 440-746, Korea, Gérard Nouet, SIFCOM UMR CNRS 6176, ENSICAEN, 6 boulevard du Maréchal Juin, 14050 Caen cedex, France

H/P.60 OPTICAL AND PHOTOELECTRONIC PROPERTIES OF MELANIN FILMS

V. Capozzi(a,b), A. Gallone(a), G. Perna(a,b), R. Cicero(c), G. Guida(c), P. Zanna(c), M. Ambrico(d) V. Augelli(b,e), P.F. Biagi (b,e), T. Ligonzo(b,e) and L. Schiavulli(b,e), (a)Dipartimento di Scienze Biomediche, Università di Foggia, Viale Pinto, 71100 Foggia, Italy, (b)Istituto Nazionale di Fisica della Materia, Unità di Bari, Bari, Italy, (c)Dipartimento di Biochimica Medica e Biologia Medica, Sezione di Biologia Medica, Facoltà di Medicina e Chirurgia, Università degli Studi di Bari, Policlinico, Bari, Italy, (d)Dipartimento di Metodologie Inorganiche e dei Plasmi del C.N.R., Via Orabona 4, 70126 Bari, Italy, (e)Dipartimento Interateneo di Fisica dell’Università di Bari, Via Amendola 173, I-70126 Bari, Italy

H/P.61 INFLUENCE OF GE AD-DIMERS ON THE CARBON INCORPORATION IN SI(001) SURFACES: A THEORETICAL STUDY

Ph. Sonnet, M. Habar, L. Stauffer, Laboratoire de Physique et de Spectroscopie Electronique, 4 rue des Frères Lumière, 68093 Mulhouse cedex, France, P.C. Kelires, Foundation for Research and Technology-Hellas (FORTH), P.O. Box 1527, 711 10 Heraclion, Crete and Physics Department, University of Crete, P.O. Box 2208, 710 03 Heraclion, Greece

H/P.62 FIRST-PRINCIPAL CALCULATIONS OF STRUCTURAL, ELASTIC AND ELECTRONIC PROPERTIES OF RO2 (R = Zr, Hf and Ce) IN FLUORITE PHASE

R. Terki, H. Faraoun, G. Bertrand and H. Aourag, Laboratoire d'Etudes et de Recherches sur les Matériaux, les Procédés et les Surfaces. LERMPS-UTBM, Belfort, France

H/P.63 ELASTIC PROPERTIES OF BINARY NiAl, NiCr AND AlCr AND TERNARY Ni2AlCr ALLOYS FROM MOLECULAR DYNAMIC AND ABINITIO SIMULATION

H. Faraoun(a), H. Aourag(a), C. Esling(b), J.L. Seichepine(a) and C. Coddet(a), (a)Laboratoire d'Etudes et de Recherches sur les Matériaux, les Procédés et les Surfaces. LERMPS-UTBM, (b)Laboratoire d'Etude des Texture et Applications aux Matériaux. ISGMP-LETAM, Belfort, France

H/P.64 AB INITIO INVESTIGATION OF THE ORDERING EFFECTS ON THE ELECTRONIC STRUCTURE OF AlN/GaN, InN/GaN AND InN/AlN SUPERLATTICES

A. Lakdja and B. Bouhafs, Modelling and Simulation in Materials Science Laboratory, Physics Department, University of Sidi Bel-Abbes, 22000 Sidi Bel-Abbes, Algeria, P. Ruterana, SIFCOM, UMR 6176 CNRS-ENSICAEN, 6 Boulevard Maréchal Juin, 14050 Caen Cedex, France

H/P.65 FIRST PRINCIPLES SEARCH FOR MULTIFERROISM IN BiCrO3

Pio Bättig and Claude Daul, Department of Chemistry, Université de Fribourg, 1700 Fribourg, Switzerland, Nicola A. Hill, Materials Department, University of California, Santa Barbara CA 93106-5050, USA

H/P.66 MODELLING OF ANISOTROPIC EXCHANGE COUPLING IN RARE-EARTH-TRANSITIONMETAL PAIRS: APPLICATIONS TO Yb^{3+}-Mn^{2+} AND Yb^{3+}-Cr^{3+} HALIDE CLUSTERS AND ITS IMPLICATION TO THE LIGHT UP-CONVERSION

M. Atanasov(a), C. Daul(b), H.U. Güdel(c), (a)Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Acad. G. Bontchev Str. Bl.11, 1113 Sofia, Bulgaria, (b)Departement de Chimie, Universite de Fribourg, Perolles, 1700 Fribourg, Switzerland, (c)Departement für Chemie und Biochemie, Universität Bern, Feiestrasse 3, 3000 Bern 9, Switzerland

H/P.67 KINETIC MONTE CARLO MODELLING OF HIGH-K ATOMIC LAYER DEPOSITION

G. Mazaleyrat, L. Jeloaica, A. Estève and M. Djafari Rouhani, LAAS-CNRS, France

H/P.68 DENSITY FUNCTIONAL THEORY OF HIGH-K REACTION MECHANISMS ON SiO_2/SI SYSTEM

L. Jeloaica, A.Dhkissi, G. Mazaleyrat, A. Estève and M. Djafari Rouhani, LAAS-CNRS, France

12:45 **LUNCH**

Thursday, May 27, 2004 Afternoon

Session VIII: Oxide materials II
Session chair: P. Hyldgaard

H-VIII.01 14:00 -Invited- HIGH-K DIELECTRICS: DEFECTS DYNAMICS FROM AB INITIO CALCULATIONS
Jacob Gavartin, Department of Physics and Astronomy, University College London, Gower street, London WC1E 6BT, U.K.

H-VIII.026 14:30 -Invited- PREDICTIVE PROCESS DESIGN: FIRST PRINCIPLES MODELLING OF ATOMIC LAYER DEPOSITION
S. Elliot, NMRC, Ireland

H-VIII.03 15:00 -Invited- MODELLING DEFECTS IN AMORPHOUS MATERIALS: AN EMBEDDED CLUSTER APPROACH
P.V. Sushko, S. Mukhopadhyay, S. Mysovsky, A. Taga, A. Shluger, Department of Physics and Astronomy, University College London, Gower St., London WC1E 6BT, U.K.

H-VIII.04 15:30 HOW MOLECULAR OXYGEN REACTS ON SILICON
N. Richard, A. Estève and M. Djafari Rouhani, CEA-DAM, Paris, LAAS-CNRS, Toulouse, France

H-VIII.05 15:45 FULLY COORDINATED SILICA NANOCLUSTERS : BUILDING BLOCKS FOR NOVEL MATERIALS
S.T. Bromley, M.A. Zwijnenburg, E. Flikkema, Lab. of Applied Organic Chemsitry and Catalysis, DelftChemTech, 136 Julianalaan, Delft University of Technology, Delft 2628 BL, The Netherlands

16:00 **BREAK**

Session IX: Semiconductor materials
Session chair: S. Elliot

H-IX.01 16:30 -Invited- ATOMISTIC MODELING OF DOPANT IMPLANTATION AND ANNEALING IN SI: DAMAGE EVOLUTION, DOPANT DIFFUSION AND ACTIVATION
Lourdes Pelaz, Departamento de Electrónica, Universidad de Valladolid, E.T.S.I. de Telecomunicación, 47011 Valladolid, Spain

H-IX.02 17:00 FIRST PRINCIPLES MODELING OF INTERMEDIATE RANGE ORDER IN AMORPHOUS SiSe2
M. Celino(a) and C. Massobrio(b), (1aCP 2400, 00100 Rome AD, Italy, (b)IPCMS, 23 rue du Loess, 67037 Strasbourg, France

H-IX.03 17:15 AB-INITIO CHARACTERIZATION OF ELECTRONIC AND OPTICAL PROPERTIES OF NOVEL ALLOY SEMICONDUCTORS
P. Palacios, J.J Fernández, P. Wahnón and C. Tablero, Instituto de Energía Solar, ETSI Telecomunicación, Universidad Politécnica de Madrid, Madrid, Spain

H-IX.04 17:30 SPATIALLY RESOLVED ELECTRICAL DEFECT SPECTROSCOPY WITH SCANNING PROBE MICROSCOPY TECHNIQUES
A. Krtschil and A. Krost, Institute of Experimental Physics, Otto-von-Guericke-University of Magdeburg, PO Box 4120, 39016 Magdeburg, Germany

H-IX.05 17:45 HALF-METALLIC Mn-DOPED SiGe ALLOYS: A FIRST-PRINCIPLES STUDY
S. Picozzi, F. Antoniella, A. Continenza, Istituto Nazionale di Fisica della Materia INFM, Dip. Fisica, Univ. L'Aquila, 67010 Coppito (Aq), Italy, A. Moscaconte, INFM-DEMOCRITOS National Simulation Center, Trieste, Italy, and SISSA, via Beirut 2/4, 34014 Trieste, Italy, A. Debernardi and M. Peressi, INFM-DEMOCRITOS National Simulation Center, Trieste, Italy, and Dip. Fisica Teorica, Univ. Trieste, 34014 Trieste, Italy

H-IX.06 18:00 A NOVEL TECHNIQUE FOR THE STRUCTURAL AND ENERGETIC CHARACTERIZATION OF LATTICE DEFECTS IN THE MOLECULAR DYNAMICS FRAMEWORK
Luis A. Marqués, Lourdes Pelaz, María Aboy, Pedro López and Juan Barbolla, Departamento de Electrónica, Universidad de Valladolid, E.T.S.I. de Telecomunicación, 47011 Valladolid, Spain

H-IX.07 18:15 NOVEL NONDESTRUCTIVE APPROACH X-RAY STANDING WAVE TECHNIQUE FOR INVESTIGATION OF Zn INCORPORATION IN III-V MATERIALS
A. Ougazzaden, Laboratoire Matériaux Optique, Photonique et Systèmes, Université de Metz / Supelec, 2 rue E. Belin, 57070 Metz, France, A.A. Sirenko, New Jersey Institute of Technology, University Heights, Newark NJ 07102-1982, USA, A. Kazimirov, Cornell High Energy Synchrotron Source (CHESS), Cornell University, Ithaca NY 14853, USA