

(24) Simulation and Modelling

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DETAILED PROGRAMME

Tuesday, 17-12-2013

Session I : 10.15 – 11.15

10.15 - 10.45 Invited Talk (1)	Arka Lahiri, Saswata Bhattacharyya, M.P. Gururajan and <u>T.A. Abhinandan</u>	ABS - Email - ICA Phase separation as a mechanism for relieving strain energy in epitaxially grown alloy thin films
10.45 - 11.15 Invited Talk (2)	<u>R. Mittal</u>	ABS - 1529 - ICA Anomalous Thermodynamic behaviour of Novel Compounds: Inelastic Neutron Scattering and Lattice Dynamics Studies

Session II : 11.45 – 13.15

11.45 - 12.15 Invited Talk (3)	<u>Kaoru Ohno</u> , Riichi Kuwahara, Shota Ono, Hotoshi Adachi, Yoshifumi Noguchi, Narcel H.F. Sluiter, Ryoji Sahara and Yoshiyuki Kawazoe	ABS - Email - ICA TOMBO, an all-electron mixed basis program
12.15 - 12.45 Invited Talk (4)	<u>Sudipta Dutta</u> and Katsunori Wakabayashi	ABS - Email - ICA Interacting Spins in Honeycomb Ribbons with Zigzag Edges
12.45 - 13.00 Oral (1)	<u>S. Bhattacharyya</u> L. T. Singh K. K. Nanda and A. K. Singh	ABS - Email - ICA Origin of Compressive Strain Induced Electromechanical Oscillations in Multiwalled Carbon Nanotubes
13.00 - 13.15 Oral (2)	Qing Chen Kaisheng Wu Gustaf Sterner Johan Bratberg Johan Jeppsson Anders Engström <u>Åke Jansson</u> Paul Mason	ABS - 206 - ICA Simulations of Precipitate Microstructure Evolution During Heat Treatment

Session III : 16.00 – 18.00

16.00 - 16.30 Invited Talk (5)	<u>Young-Woo Son</u>	ABS - Email - ICA Origin of anomalous water permeation through graphene oxide membrane.
16.30 - 17.00 Invited Talk (6)	Vinay Kandagal, Tonnishtha Das Gupta, Sudeep Punnathanan, Amardeep Pathak and <u>K.G. Ayappa</u>	ABS - Email - ICA Functionalizing Graphene Nanoribbons for Improved Methane and Carbon dioxide Gas Storage

17.00 - 17.30 Invited Talk (7)	<u>Hisato Yasumatsu</u>	ABS - Email - ICA Electron Accumulation at Sub-Nano Interface by Dosing of Uni-Size Pt Cluster Disk on Si(111) Surface and its Application to Catalytic CO Oxidation
17.30 - 17.45 Oral (3)	<u>Moumita Mukherjee</u> and D. N. Bose	ABS - 1657 - ICA IV-IV and III-V WBG Semiconductors as New Sources for Terahertz Power Generation
17.45 - 18.00 Oral (4)	<u>S. Q. Wang</u>	ABS - 362 - ICA Car-Parrinello Molecular Dynamics Simulation of Graphene Sheets

Wednesday, 18-12-2013

Session IV : 10.15 – 11.15

10.15 - 10.45 Invited Talk (8)	<u>Y.Y. Liang</u>	ABS - Email - ICA All Carbon Mackay-Like crystals with 8-fold symmetry
10.45 - 11.00 Oral (5)	<u>Shanti Swaroop Sharma</u> Ankit Sahai Rahul Swarup Sharma and K. HansRaj	ABS - 497 - ICA Influence of process parameters in multi-pass Twist Extrusion of Cu99
11.00 - 11.15 Oral (6)	<u>M. Srinivasan</u> and P. Ramasamy	ABS - 532 - ICA Directional solidification crystal growth processes for PV cells: Numerical simulation on Marangoni convective flow of the silicon melt

Session V : 11.45 – 13.15

11.45 - 12.15 Invited Talk (9)	<u>Manish Jain</u>	ABS - Email - ICA New Methods to Accelerate GW Calculations
12.15 - 12.30 Oral (7)	<u>R. Mukherjee</u> D. Molnar A. Mora P. Binkele A. Choudhury S. Schmauder and B. Nestler	ABS - 1414 - ICA Multiscale Modelling of Coarsening in Fe-Cu Alloy using Kinetic Monte Carlo, Molecular Dynamics and Phase-field Simulations
12.30 - 12.45 Oral (8)	<u>Sanjay Tiwari</u> Sue A. Carter and Campbell Scott	ABS - 827 - ICA Electrical modelling of Multilayer Organic Light emitting diodes

Poster Session:

Wednesday, 18-12-2013, 14.00 - 15.30

24 - Poster - 01	Paramita Dutta Santanu K. Maiti and S. N. Karmakar	Renormalization-group method for persistent current in a finite width quasiperiodic ring ABS - 122 - ICA
24 - Poster - 02	I. Sinha and R. K. Mandal	Isothermal nanocrystallization kinetics adaptation of the KJMA model ABS - 129 - ICA

24 - Poster - 03	Santanu K. Maiti	Conformation-dependent electron transport through a biphenyl molecule: Verification of experimental results	ABS - 135 - ICA
24 - Poster - 04	Santanu K. Maiti Moumita Dey and S.N. Karmakar	Quantum Hall Effect: A Lattice Model	ABS - 180 - ICA
24 - Poster - 05	G. Tiwari M.A. Iqbal and P.K. Gupta	Numerical Simulation of Penetration and Perforation Behavior of Thin Aluminum Layered Target Subjected to Oblique Impact	ABS - 213 - ICA
24 - Poster - 06	S. Q. Wang	Modeling the Paracrystalline Structure of High-entropy alloys	ABS - 362 - ICA
24 - Poster - 07	Atul Dayal Rahul Swarup Sharma K. Hans Raj	Study of Processing Routes in Equal Channel Angular Pressing of Aluminium Alloy (Al-6082) using Finite Element Analysis.	ABS - 400 - ICA
24 - Poster - 08	Sangeeta Khare and Puneet Mahajan	Effect of Mn and Si on growth kinetics of ferrite in Fe-C-X alloys	ABS - 528 - ICA
24 - Poster - 09	P Kartheek Ahmad Omar and K Narasimhan	Effect of bi-linear strain paths on forming limit strain	ABS - 629 - ICA
24 - Poster - 10	Mamta Khaneja Santanu Ghosh P.K. Chaudhury Vikram Kumar	Simulation of Field Emission Behaviour from Multiple Carbon Nanotubes in Integrated Grid Triode Configuration	ABS - 724 - ICA
24 - Poster - 11	S. B. R. Devireddy and S. Biswas	The Effect of Interphase on Mechanical and Thermal Properties of Glass Fiber Reinforced Epoxy Composites	ABS - 795 - ICA
24 - Poster - 12	N Subramanya Vijay Kumar Sutrakar and D Roy Mahapatra	Molecular Dynamic Mechanism of Crack Initiation and Propagation in Nano-crystalline Aluminum	ABS - 810 - ICA
24 - Poster - 13	M Javeed Akhter Vijay Kumar Sutrakar and D Roy Mahapatra	Post-Shock Compression Behaviour of Nano-Structured Copper	ABS - 810a - ICA
24 - Poster - 14	Ganesh Iyer Arun Kumar and Anandh Subramaniam	Stability of Interfacial Misfit Dislocation in Superlattices	ABS - 1108 - ICA
24 - Poster - 15	Srinivasan. N Ravi Kumar R.Velmurugan S.K. Singh, Bhanu Pant	Microstructural investigation of Ti-6Al-4V under biaxial stress state using cruciform specimen geometry	ABS - 1109 - ICA
24 - Poster - 16	Manjunath GA Sambhav Galada Eeshaanee Arya Mohit Garg M.N. Vijayaraghavan K.N. Bhat Navakanta Bhat	Modeling, Simulation and Characterization of Silicon Nanowires	ABS - 1115 - ICA

24 - Poster - 17	Marrapu Bhargava Shanta Chakrabarty Asim Tewari and Sushil K. Mishra	Formability studies for Transformation Induced Plasticity (TRIP) steels	ABS - 1239 - ICA
24 - Poster - 18	Shanta Chakrabarty Marrapu Bhargava Prita Pant and Sushil K. Mishra	Determination of strain path diagram and evolution of microstructure at different strain and strain path for low-Ni austenitic stainless steel	ABS - 1242 - ICA
24 - Poster - 19	Somnath Bhowmick and Jan Ruzs	How Efficient is Electron Vortex Beam for Magnetic Characterization?	ABS - 1258 - ICA
24 - Poster - 20	Vineet Tiwari and Geetika Srivastava	Optimal Design of Polymer Based Piezoelectric Actuator with Varying Thickness & Length Ratios	ABS - 1320 - ICA
24 - Poster - 21	Rajeev S. Joshi D. Venkateswarlu and P. S. Anil Kumar	Micromagnetic Simulation of Static Magnetic Properties and Effect of Using the Mirrored Mesh in Finite Element Method	ABS - 1355 - ICA
24 - Poster - 22	Puneet Kumar and Dr. J. Srinivas	Study of Dynamic and Buckling Characteristics of Carbon Nanotube Reinforced Polymer Nanocomposites	ABS - 1415 - ICA
24 - Poster - 23	Arijit Roy and M.P. Gururajan	Phase eld modelling of microstructural evolution using interfacial energy anisotropy parameters obtained from molecular dynamics simulations	ABS - 1513 - ICA
24 - Poster - 24	Prachi Limaye Saransh Singh M P Gururajan and Prita Pant	Effect of Stacking Fault Energy on the Deformation Behaviour of FCC Metals and Alloys	ABS - 1519 - ICA
24 - Poster - 25	Kartik Sau and P. Padma Kumar	Molecular Dynamics Investigation of Na ⁺ in Na ₂ Ni ₂ TeO ₆	ABS - 1546 - ICA
24 - Poster - 26	Naveen Kumar T.A. Abinandanan1	Percolation of Phases during Spinodal Decomposition in Ternary Systems	ABS - 1548 - ICA
24 - Poster - 27	Anand Dutt Mira Mitra and M.P. Gururajan	Wavelet Galerkin Solution to Cahn Hilliard and Allen Cahn Equation	ABS - 1569 - ICA
24 - Poster - 28	Gudipadu Venkatesh Appurba Kumar Sharma and Nitish Singh	Simulation of Ultrasonic Assisted Abrasive Flow Machining Process	ABS - 1586 - ICA
24 - Poster - 29	B. Ghosh S. Halder and T.P. Sinha	Vibrational modes and first principles study of double-perovskite A ₂ SmTaO ₆ (A= Ba, Sr, Ca)	ABS - Email - ICA
24 - Poster - 30	Aaditya Manjanath Vijay Kumar and Abhishek K. Singh	Mechanical and electronic properties of pristine and Ni-doped Si, Ge and Sn sheets	ABS - Email 1 - ICA
24 - Poster - 31	Deya Das Rahul P. Hardikar Sang Soo Han Seungchul Kim Kwang-Ryeo Lee and Abhishek K. Singh	Boron doped defected graphene: A promising anode material for Li ion battery	ABS - Email 2 - ICA