Oral presentations

Monday, July 19

8:00–10:00 Registration

8:50–9:00 Conference opening

Session 1: Potentials and novel approaches, Chair: Kai Nordlund

9:00 I1 Atomistic-scale Simulations of Chemical Reactions: Bridging from Quantum Chemistry to Engineering
Michael F. Russo Jr., Adri C. T. van Duin

9:40 O1 Evaluation of a New Bond-order Potential for Si
Matthias Posselt

10:00 O2 A Modified Interatomic Potential for Tungsten-hydrogen System with Defects and the Hydrogen Diffusion Behaviors
Xiaolin Shu, Xiao-Chun Li, Yi-Nan Liu, F. Gao, Wangyu Hu, Guang-Hong Lu, Tianmin Wang

10:20 O3 Mixed Resolution Model of C_{60} Cluster Bombardment
Paul E. Kennedy, Barbara J. Garrison

10:40–11:00 Coffee break

Session 2: Cluster bombardment I, Chair: Herbert Urbassek

11:00 I2 Experimental Studies of Energetic Cluster/Solid Interactions – Synergy with Computer Simulations
Nicholas Winograd

11:40 O4 Desorption of Large Molecules with Light-element Clusters: Effects of Cluster Size and Substrate Nature
Arnaud Delcorte, Barbara J. Garrison

12:00 O5 Sensitivity Analysis of Crater Formation on the Energy Deposition of keV Clusters on Molecular Solids
Jaydeep D Mody, Roger P Webb

12:20 O6 Modeling of Thermal Sputtering Due to CO_2 Cluster Impact on Carbon-based Surfaces
Yasutaka Yamaguchi, Tomohiro Shinya, Hisato Yasumatsu

12:40–14:00 Lunch

Session 3: Cluster bombardment II, Chair: Arnaud Delcorte

14:25 O7 MD Simulation of Huge Reactive Gas Cluster Impact with Supersonic Velocity
Takaaki Aoki, Toshio Seki, Jiro Matsuo

14:45 O8 Erosion of Ag Surface by Continuous Irradiation with Slow, Large Ar Clusters
Lukasz Rzeznik, Robert Paruch, Barbara J. Garrison, Zbigniew Postawa

15:05 O9 Fluence Effects in C_{60} Bombardment of Si
Kristin D. Krantzman, Barbara J. Garrison

15:25 O10 Interaction of Energetic Clusters (Au_3, Au_{400} and C_{60}) with Organic Material and Adsorbed Gold Nanoparticles
Oscar A. Restrepo, Arnaud Delcorte

15:45 O11 Radiation Effects of Copper Singles Crystals
Masao Doyama, Y. Kogure, T. Nozaki

16:05–16:30 Coffee break

Session 4: Surface phenomena/Topography, Chair: Takaaki Aoki

16:30 O12 The Sputtering Cross-section of a Surface-vacancy Island
Yudi Rosandi, Herbert M. Urbassek

16:50 O13 Surface Topography Induced by Swift Ion Impacts
Chris Scott, Roger Smith

17:10 O14 Molecular Dynamics Simulation of Ripple Growth in the Presence of Fe Contamination in Si
Peter Süle

17:30 O15 Modelling High Thermal Loads, Sputtering and Tritium Retention in Diamond for Fusion Applications
Alastair Dunn, Dorothy Duffy

17:50 O16 Binary Collision Simulation of Focused Ion Beam Milling of Deep Trenches
Gerhard Hobler, Dalibor Kovac

19:15 International Advisory Committee meeting (Conference room at the second floor).

Tuesday, July 20

Session 5: Electronic stopping, Chair: Fei Gao

9:00 I3 Quantum Mechanical Simulations of Electronic Stopping in Metals
W.M.C. Foulkes, M.W. Finnis, A.P. Horsfield, J. le Page, D.R. Mason, C.P. Race, A.P. Sutton

9:40 O17 Electronic Effects in Radiation Damage Simulations in Metals and Insulators
Dorothy Duffy, Jack Mulroue, Szymon Daraszewicz

10:00 O18 Molecular Dynamics Study of Si Sputtering and Track Formation in Swift Ion Interactions with Amorphous SiO_2
S. Mookerjee, O. Pakarinen, F. Djurabekova, K. Nordlund, M. Toulemonde, A. Roy

10:20 O19 Simulation of Sputtering of a Multilayer Molecular Solid by MeV Ion Impact
Roger P Webb, Jaydeep D Mody

10:40–11:00 Coffee break

Session 6: Emission of electrons and ions, Chair: Nicholas Winograd

11:00 I4 Ion Induced Electronic Excitation of Solids: Model Calculations and Experiment
A. Wucher

11:40 O20 Modeling Kinetic Electron Emission with Molecular Dynamics
A. Duvenbeck, S. Hanke, B. Weidtmann, A. Wucher

12:00 O21 Secondary Electron Emission Yield Calculation Performed Using Two Different Monte Carla Strategies
Maurizio Dapor

12:20 O22 Molecular Ions in C_{60} Bombardment of Solids
Barbara J. Garrison

12:40–14:00 Lunch

Session 7: Photon/electron stimulated processes, Chair: Barbara J. Garrison

14:25 I5 Atomic-level Simulations of Laser Interactions with Metals: Mechanisms of Melting and Resolidification, Generation of Crystal Defects
Leonid V. Zhigilei, Zhibin Lin, Eaman Tahir Abdul Karim, Chengping Wu

15:05 O23 Molecular Dynamics Simulations of Matrix Assisted Laser Desorption Ionization: Analysis of Intermolcular Matrix-analyte Interactions
Shivangi Nangia, Barbara J. Garrison

15:25 O24 Atomic Mixing and Structural Transformations in Ag/Au Film – Cu Substrate Systems Irradiated by Femtosecond Laser Pulses
Chengping Wu, Derek A. Thomas, Zhibin Lin, Leonid V. Zhigilei

15:45 O25 Orientation Dependence of Near-threshold Damage 4H Production by Electron Irradiation of 4H SiC and Diamond
J. W. Steeds

16:05–16:30 Coffee break

Session 8: Semiconductors, Chair: Matthias Posselt

16:30 I6 Diffusion Phenomena in Isotopically Controlled Semiconductor Heterostructures
Hartmut Bracht

17:10 O26 Optimization of Amorphous Silicon and Silica Structures for Molecular Dynamics Simulations
Juha Samela, Scott A. Norris, Kai Nordlund, Michael J. Aziz

17:30 O27 Low-energy Oxygen Bombardment of Silicon by MD Simulations Making Use of a Reactive Force Field
P. Philipp, L. Briquet, T. Wirtz, J. Kieffer

18:00–20:00 Poster session I (odd-numbered posters)

Wednesday, July 21

Session 9: Nanoscience (joint session with ICACS24), Chair: Roger Webb and Peter Sigmund

9:00 I7 Interaction of Charged Particles with Insulators and Living Cells
Y. Yamazaki

10:10 I8 Ion Beam Modification of Nanocrystals: Simulation and Experiment
Flyura Djurabekova, Kai Nordlund

10:55–11:20 Coffee break

Session 10: Nanostructures, Chair: Marc Hou

11:20 O28 Threshold Defect Production in Mechanically Strained Single-walled Carbon Nanotube and Silicon Nanowire
E. Holmström, L. Toikka, A. V. Krasheninnikov, K. Nordlund

11:40 O29 The Effect of Helium Bubble on the Mechanical Properties of Palladium Nanowire
Liang Wang, Wangyu Hu, Huiqiu Deng, Xiyuan Yang, Xiaojun Cui

12:00 O30 Mechanism of Selective Nano Structure Formation on Pre-patterned Surfaces
Satoshi Numazawa, Karl-Heinz Heinig

12:20 O31 Structure of Si/Ge Nanoclusters as Studied by Molecular Dynamics and Semi-Grand-Canonical Monte Carlo Methods
Ari Harjunmaa, Kai Nordlund, Alexander Stukowski, Karsten Albe

12:40 O32 Nanoscale Phase Transitions within Swift-heavy Ion Tracks in Pyrochlore Structures
William J. Weber, Ram Devanathan, Jiaming Zhang, Maik Lang, Rodney C. Ewing, Marcel Toulemonde

13:00–14:00 Lunch

16:15 Conference outing to the Wieliczka Salt Mine

19:00 Conference dinner at the Wieliczka Salt Mine

Thursday, July 22

Session 11: Materials for nuclear and fusion industry I, Chair: Maria Caturla

9:00 I9 Multiscale Viewpoint of Radiation Damage Process in Fusion Materials
Kazunori Morishita, Junichi Yoshimatsu, Yasunori Yamamoto, Yoshiyuki Watanabe

9:40 O33 He Bubbles Growth Mechanism in FeCr
Alfredo Caro, A. Stukowski, P. Erhart, B. Sadigh, M. Caro

10:00 O34 Towards Suppressing Blistering by Investigating Physical Origin of Hydrogen/Helium Interactions with Tungsten
Guang-Hong Lu, Hong-Bo Zhou, Yue-Lin Liu, Shuo Jin, Ying Zhang, G. -N. Luo

10:20 O35 Microstructure Evolution of He-irradiated Tungsten: an OKMC Model Using Ab Initio Calculations for Diffusion Parameters and Binary Collision Approximation for Slowing Down of He Atom
C.S. Becquart, C. Domain, U. Sarkar, A. DeBacker, M. Hou

10:40–11:00 Coffee break

Session 12: Materials for nuclear and fusion industry II, Chair: Alfredo Caro

11:00 O36 IAEA Activities on R&D of Structural Materials for Advanced Reactor Systems
A. Zeman, N. Dytlewski, G. Mank

11:20 O37 Radioparagenesis: the Effects of Transmutation on Crystalline Stability
C.R. Stanek, C. Jiang, N.A. Marks, K.E. Sickafus, B. P. Uberuaga

11:40 O38 Molecular Dynamics Study of Damage Production in Uranium Dioxide Under Irradiation
Guillaume Martin, Catherine Sabathier, Philippe Garcia, Laurent Van Brutzel, Serge Maillard

12:00 O39 Interaction of Carbon with Point Defect Clusters in α-Fe: an MD Study
V. Jansson, D. Terentyev

12:20 O40 Multi-scale Modeling of Irradiation Effects in Spallation Neutron Source Materials
Toshimasa Yoshiie, Takahiro Ito, Hiroshi Iwase , Yoshihisa Kaneko, Masayoshi Kawai, Ippei Kishida, Satoshi Kunieda, Satoshi Shimakawa, Futoshi Shimizu, Satoshi Hashimoto, Naoyuki Hashimoto, Tokio Fukahori, Yukinobu Watanabe, Shiori Ishino

12:40–14:00 Lunch

Session 13: Metals and alloys I, Chair: Anna Zurek

14:25 I10 Multi-time Scale Modeling of Radiation Damage at Grain Boundaries
Xian-Ming Bai, Arthur F. Voter, Richard G. Hoagland, Michael Nastasi, Blas P. Uberuaga

15:05 O41 Microstructure Evolution of Irradiated Fe on the Presence of He Studied by Kinetic Monte Carlo
Maria J. Caturla, C. C. Fu

15:25 O42 Structure and Stability of Σ5 (210) and Σ3 (111) Grain Boundaries in Iron
Tomasz Ossowski, J. Kuriplach, E.E. Zhurkin, M. Hou, A. Kiejna

15:45 O43 Study of Irradiation Induced BCC Nb Precipitates in the Zr-Nb Alloy by Ab Initio Calculations and Molecular Dynmics Simulations
X. K. Xin, W. S. Lai

16:05–16:30 Coffee break

Session 14: Ceramics, Chair: William J. Weber

16:30 I11 Effects of Charges and Charge Transfer on Defects and Defect Generation in Ceramics
Fei Gao, H. Y. Xiao, W. J. Weber

17:10 O44 Calculation of Proper Vacancy Migration Energy Barriers with Artificial Neural Networks for the Modelling of Vacancy Clusters' Migration
N. Castin, L. Malerba

17:30 O45 Molecular Dynamics Simulation of Threshold Displacement Energies in Lithium Aluminate
Hiroki Tsuchihira, Takuji Oda, Satoru Tanaka

17:50–19:50 Poster session II (even-numbered posters)

20:00 Concert at the Auditorium Maximum

Friday, July 23

Session 15: Long timescale simulations, Chair: Toshimasa Yoshiie

9:00	I12	Long Timescale Modelling of the Growth of Rutile *L.J. Vernon, S. Blackwell, S. D. Kenny, R. Smith*
9:40	O46	Long Time Radiation-induced Defect Diffusion in Ionic Systems *Lanchakorn Kittiratanawasin, Roger Smith*
10:00	O47	Multiphysics Program for Ion-Induced Collision Cascades and Thermally Activated Phase Separation: Intermetallic Nanolayers by Interface Mixing *Bartosz Liedke, K.-H. Heinig, S. Facsko, W. Möller*
10:20	O48	Microstructural Evolution of Iron in Radiation Environment *A. Souidi, M. Hou, C.S. Becquart, C. Domain, L. Malerba, R. E. Stoller*
10:40–11:00		Coffee break

Session 16: Metals and alloys II, Chair: Roger Smith

11:00	O49	Theoretical Calculations for Magnetic Property of FeRh Inter-metallic Compound Irradiated with Energetic Ions *Yasunori Kaneta, Akihiro Iwase, Shuichi Iwata*
11:20	O50	Effect of Cr on the Behavior of He in FeCr Alloys From First Principles *Chu Chun Fu, E. Martinez, R. Soulairol*
11:40	O51	Defect Kinetics in Carbon-doped α-Iron: a Multiscale Modeling *T. Jourdan, C. C. Fu, L. Joly, J.-L. Bocquet, M. J. Caturla, F. Willaime*
12:00	O52	The Influence of Stress on Primary Defect Damage by Displacement Cascades in BCC Iron *K. P. Boyle, Ishraq Shabib, R. E. Miller*
12:20	O53	Nucleation of Cu-vacancy and Ni-vacancy Clusters in BCC-Fe *A.T. Al-Motasem, M. Posselt, F. Bergner*
12:40–13:00		Closing of the conference
13:00–14:00		Lunch