

ORAL PRESENTATIONS : PROVISIONAL PROGRAMME (SUBJECT TO CHANGE)

Monday 20th June 2016

8-50 Opening

Particle-surface interactions

9-00

I1 H. Urbassek [Sputtering of curved surfaces](#)

01 G. Hobler [Vienna](#) [Sputtering of silicon membranes with nanoscale thickness](#)

02 A. Lloyd [Loughborough University](#) [Modelling Ag thin film growth on ZnO](#)

03 V. Jansson [Helsinki](#), [Kinetic Monte Carlo simulations of the long-term metal surface evolutions](#)

04 M. Golunski [Computer Modelling of Ejection of Phenylalanine Molecules Deposited on Free-Standing Graphene by keV C₆₀ Projectiles](#)

10-50

break

11-10

I2 Barbara Garrison, [PSU](#) [Effect of Oxygen Chemistry in Sputtering of Polymers](#)

05 C. Anders, [Kaiserslautern](#) [Formation of molecular products after keV-ion impact in cosmic ice surfaces](#)

06 A. Lopez-Cazalilla [Helsinki](#), [Nanoripples production on a-Si and a-Ge surfaces under Ar irradiation](#)

07 S. Norris [PyCraters: A Python framework for crater function analysis](#)

08 Udo von Toussaint [Efficient Uncertainty Quantification for computer simulations of ion-solid interactions: the effect of multiple uncertain inputs on sputtering and reflection](#)

13-00

Lunch

14-00

I3 E. Vittone [Modelling of charge collection efficiency degradation in semiconductor devices induced by MeV ion beam irradiation](#)

09 P. Philipp [Modifications in polymers due to the irradiation with light rare gas ions](#)

010 D. Maciazek [Poland](#), [Computer Simulations of \(CO₂\)₂₀₀₀ and Ar₂₀₀₀ Impacts at Polystyrene Sample](#)

011 J. Guérolé [Erlangen-Nurnberg \(FAU\)](#), [Irradiation damage induced eigenstrains in metals and ceramics: an atomistic simulations of focussed ion beam machining](#)

15-30

break

Nanomaterials

- 16-10 013 E. Baibuz, Helsinki, Formation Mechanism of Iron Nanocubes in Magnetron Sputtering Inert Gas Condensation
014 F. Valencia, Chile, Irradiation of hollow nanoparticles
015 . R. I. Gonzales, Santiago, Chile, Metal Nanotube composites as radiation resistant materials.
P35 M. Bhatnagar, FCIPT, Gujarat, India Molecular Dynamics study of growth and thermal dynamics of Ag clusters on a nano rippled SiO₂ surface
- 17-30 end

Tuesday 21st June 2016

Electronic energy loss and ion tracks

- 9-00 023 A. Correa LLNL, USA An ab initio model of the electron-phonon interaction within classical molecular dynamics
017 G. Khara Modelling swift heavy ion irradiation of silicon using atomistic two temperature molecular dynamics
018 A. Prada Madrid Ion irradiation-induced high electronic excitation in silica: bulk and surface analysis by means of atomistic simulations
019 A. Tamm Estonia Coupling electrons with lattice vibrations within classical molecular dynamics
020 R. Rymzhanov Dubna, Modelling transient non-equilibrium electronic and atomic kinetics after high energy deposition in semiconductors and dielectrics
Russia

10-50 break

- 11-10 I5 Dorothy Duffy, UCL, UK, Coupled effects of nuclear and electronic energy loss in radiation damage
021 A. Adrych-Brunning- Manchester, Primary damage induced in zirconium alloys
022 S. Murphy UCL *The role of electronic excitation on the structural evolution of laser irradiated nano films*

Nanostructure and defect evolutions

027 Fei Gao Michigan EVOLUTION OF NANOSIZE DEFECTS TO EXPERIMENTALLY RELEVANT TIME SCALES

13-00 Lunch

14-00

I6 D. Mason UK scaling and elastic interaction between defects formed in collision cascades: observations and simulations

in the timescale gap

025 M.J. Caturla Alicante_DYNAMIC MODIFICATION OF DISLOCATIONS FROM NEARBY COLLISION CASCADES

026 T. Nakasuji Kyoto, Japan, Monte-Carlo simulation of defect-cluster nucleation in metals during irradiation

P51 Tom Swinburne CULHAM *Fast, vacancy-free climb of prismatic dislocation loops in bcc metals*

028 Enrique Martinez Los Alamos, Thermal Activation of Dislocations in Large Scale Obstacle Bypass

15-30

break

16-10

029 Monica Chiapetto SCK-CEN Belgium, *Development of an object kinetic Monte Carlo model for the microstructure evolution of neutron-irradiated reactor pressure vessel steels*

030 B. Pannier EDF France Development of an AK Monte Carlo model to simulate the long-term microstructural evolution of pressure vessel steel under irradiation

031 B. Liedke HZDR Germany, Kinetic Monte Carlo simulation of irradiation-induced nanostructure evolution in Oxide Dispersion Strengthened Fe alloys

032 I. Dopico, Getafe Spain A KINETIC MONTE CARLO STUDY OF IRRADIATED IRON IN FUSION ENVIRONMENTS: DIFFERENCES BETWEEN MODES OF IRRADIATION

17-30

end

Wednesday 22nd June 2016

9-00

17 K. Arakawa, Shimane University, Japan TEM of dynamics of radiation-produced defects in metals: comparison with simulations

033 K. Morishita Kyoto Evaluation of energetics of copper-vacancy clusters in Fe

034 N. Castin, Belgium Artificial Neural Network based cohesive model from ab initio: principles and applications to single point-defect migration in binary Fe-based alloys

Covalent Materials

035 N. Marks, Australia, Radiation Damage Cascades in Diamond

036 T. Trevethan Surrey, Atomistic Models of Polycrystalline Nuclear Graphite

10-50 break
11-10 I8 Lourdes Pelaz, [Bridging radiation induced defects to macroscopic effects through multiscale modelling](#)

Fe-Cr and alloy Systems

037 . I. Dopico [Murcia, Spain](#), KINETIC MONTE CARLO SIMULATION OF PHASE-PRECIPIATION VERSUS INSTABILITY BEHAVIOUR IN SHORT PERIOD FeCr SUPERLATTICES

038 M. Zemła [Warsaw, Poland](#) Helium embrittlement of grain boundaries in Fe-Cr alloys

039 Kunok Chang [Phase field modelling of MN-NI-Si precipitate behaviour in RPV steel](#)

040 Flyura Djurabekova [University of Helsinki](#) Mechanism of Reduced Radiation Damage Identified in Complex Alloys

13-00 Lunch

Fusion materials 1: Beryllium

14-20 041 Paul Fossati [Imperial College](#), Radiation Damage in Beryllium

043 P. Vladimirov [KIT Germany](#), Ab initio study of the threshold displacement energy in beryllium

044 C. Stihl [Karsruhe, Germany](#), Modelling tritium on the beryllium-(0001)-surface

Nanomaterials

016 E. Bringa [Argentina](#) Coupling of irradiation and mechanical properties in nanostructured materials

15-40 Poster Session

Thursday 23rd June 2016

Waste Forms

9-00 I9 A. Saul CEA [Radiation damage in cement](#)

042 YAQI JI [Juelich, Germany](#), COMPLEMENTARY ATOMISTIC MODELLING AND EXPERIMENTAL STUDIES OF RADIATION DAMAGE IN MONAZITE-TYPE CERAMIC NUCLEAR WASTE FORMS

045 Piotr M. Kowalski [Juelich](#), Simulation of ceramic materials relevant for nuclear waste management

046 G. Adjanor [EDF France](#) Sink-strengths calculations for mixed 1D-3D mobile species

Cascades

047 J.P. Crocombette [Molecular dynamics simulations of high energy cascade in ordered alloys : defect production and subcascade division](#)

10-50 break

11-10 I10 Yonggang Li, [Hefei, China, Computer Simulation of Primary Radiation Damage and Long-term Evolution of Defects in Nuclear Structural Materials](#)

048 M.R. Gilbert, [Culham, UK Nuclear physics applications to materials modelling: transmutation and primary damage events](#)

049 T. Yoshiie [Kyoto, Reaction Rate Analysis of Defect Structures in Test Pieces of Reactor Pressure Vessel](#)

050 Aliz Simon, [IAEA, Cross-cutting Research & Development on Radiation Effects in Materials](#)

051 B. J. Braams [IAEA, Vienna Activities at IAEA on data for plasma-material interaction in fusion devices and related material properties](#)

13-00 Excursion to Newton's birthplace (packed lunch)

18-30 Conference dinner

Friday 24th June 2016

Fusion Materials 2: TUNGSTEN

9-00 I11 Luis Sandoval, [AMA, Inc., NASA-ARC, USA, Nucleation and Growth of Helium Bubbles in Tungsten: Long Timescale Simulations](#)

052 Guang-Hong Lu [Beihang University, Beijing Atomistic mechanism of shear-coupled grain boundary migration in W: effects of H and He](#)

053 Petr Grigorev, [Belgium On the mechanisms of hydrogen retention in tungsten: an atomistic approach](#)

054 E. A. Hodille, [CEA France Simulation of hydrogen isotopes trapping in tungsten by irradiation-induced traps](#)

055 Alexander Bakaev [Belgium Trapping of hydrogen and helium at dislocations in tungsten: an ab initio study](#)

10-50 break

11-10 056 Li-Fang Wang [China A new EAM interatomic potential for tungsten-hydrogen system](#)

057 A. Rivera Universidad Politécnica de Madrid coarse-grained and nanostructured tungsten under ion irradiation for nuclear fusion feasibility studies: An object kinetic Monte Carlo description

058 Y.H. Li Beihang, China, Interstitial-mediated diffusion and clustering for transmutation elements Re and Os precipitation in W

059 J. Fikar Republic Interaction of Irradiation Induced Prismatic Dislocation Loops with Free Surfaces in Tungsten

060 J.S. Wrobel Warsaw Phase stability of irradiated W-Re Solid Solution

12-30

End of meeting.

COSIRES POSTERS

1. Xiaolin Shu Beihang University, Beijing 100191, China The tungsten cluster structure by Molecular dynamics simulation

***2. Rebecca Bird, Birmingham University, Atomistic Simulation of CeTi₂O₆ - A Candidate Ceramic for the Immobilization of High Level Waste

*****3. Flyura Djurabekova University of Helsinki Interaction of swift heavy ions with three- and two-dimensional materials **now oral**

P3 Ruslan Rymzhanov Dubna Russia, Effect of model cross sections on excitation of the electronic system in tracks of swift heavy ions in solids

4. Baoqin Fu Sichuan University, Chengdu 610065, PR China Molecular Dynamics Study of the Dislocation Effect on displacement cascade in Tungsten

5. Xiao-Chun Li Chinese Academy of Sciences, Hefei Atomistic study of hydrogen behaviour around a screw dislocation in alpha iron

6. Alejandro Prada Universidad Politécnica de Madrid Molecular dynamics simulation of embedded silver nano-particles in silica: elongation analysis

7. Amal Alharbi Loughborough, Interaction potentials for modelling borosilicate glass

8. A. Dubinko Nuclear Materials Science Institute, Boeretang 200, Belgium Effect of high flux plasma exposure on micro-structural and -mechanical properties of poly- and single crystal tungsten

9. Blas Pedro Uberuaga LANL, Accelerated molecular dynamics studies of cation kinetics in pyrochlore

10. C. V. S. Brahmmananda Rao, IGCAR, India, ELECTRONIC STRUCTURE AND COMPLEXATION BEHAVIOUR OF DI-n-ALKYL H-PHOSPHONATES

11. C. Anders, Kaiserslautern, Crater production by nano-cluster impact on Au nanofoams
12. Eleni Chatzikyriakou, University of Southampton, Finite Elements Method simulation of leakage path formation in 22 nm bulk FinFETs under Total ionizing Dose
13. Emma del Rio Universidad Politécnica de Madrid, Madrid STABILITY OF VACANCY LOOPS CLOSE TO SURFACES IN α -Fe FROM MOLECULAR DYNAMICS SIMULATIONS
14. F. Gao Michigan Computer Simulation of Displacement Damage and Effective NIEL in GaAs
15. F. Valencia, Chile, Confinement effects on Nanocrystalline Diamond: Bulk and Surface effect
16. Fredric Granberg Helsinki, Multiscale Modelling of Dislocation Interactions with Obstacles
17. Malcolm I. Heggie Surrey DEDUCTIONS ABOUT RADIATION DAMAGE IN GRAPHITE FROM MOLECULAR DYNAMIC RESULTS
18. Gerhard Hobler TU Wien Simple model of surface roughness for binary collision sputtering simulations
19. Huiqiu Deng Hunan China, Microstructure evolution of Cu-Zr metallic glass under neutron irradiation
20. Ignacio Dopico Getafe, Spain MULTISCALE MODELLING OF THE EVOLUTION OF FeCr ALLOYS: FROM ATOMISTIC SIMULATIONS TO MECHANICAL PROPERTIES
21. J. S. Wróbel Warsaw Point defect properties of ternary Fe-Cr-Ni alloys
22. J. Abujas-Pereira A Distributed-Memory Parallel Lattice Kinetic Monte Carlo Algorithm for Crystal Growth Applied to Barite (001) Face Cadiz, Spain
23. Juan Liu Tsinghua University, China OXIDATION BEHAVIOR OF BORON DOPED IRRADIATED GRAPHITE BY FIRST PRINCIPLES THEORY
24. Michal Kanski, Kraków, Poland Sputtering of Octatetraene Samples by C60 Projectiles: Comparison of Reactive Interatomic Potentials
25. K. Nordlund, Helsinki, Major channelling effects on sputtering of nanowires
26. Kenny Jolley, Radiation tolerance of iron phosphate: A study of amorphous and crystalline structures
27. Liang-Liang Niu, Energetics of vacancy segregation to [100] symmetric tilt grain boundaries in bcc W
28. Manan Dholakia, Development of empirical interatomic potentials for Y2TiO5 and Y2Ti2O7 and study of displacement cascades using Molecular Dynamics
29. A. De Backer, Culham, Hydrogen interaction with interstitial type defects predicted by Molecular Dynamics and Density Functional Theory
30. M.J. Wooton, Loughborough, Radiation Damage in Advanced Materials for Next Generation Nuclear Power Plants
31. Martin Mainitz, Kaiserslautern Irradiation of astrophysical ice grains by cosmic-ray ions: a REAX simulation study
32. M. Posselt, First-principles-based calculation of self- and solute diffusion in bcc-Fe

33. Juan Carlos Moreno-Marín, Alicante, Spain, Electronic energy loss of swift carbon atoms after traversing carbon nanostructures
34. Juan Carlos Moreno-Marín Alicante, Spain Efficiency of multiwalled carbon nanotubes as masks against carbon or argon irradiation
- *****35. M. Bhatnagar, FCIPT, Institute for Plasma Research, Gujarat, India Molecular Dynamics study of growth and thermal dynamics of Ag clusters on a nano rippled SiO₂ surface **Now oral**
36. Pengbo Zhang Dailan, China, Diffusion and retention of hydrogen in V in presence of Ti and Cr
- ***37. R. Alexander, CEA France, The ab-initio energetics of large interstitial clusters in body centred cubic metals: application to Fe, W, V and Ta **Poster withdrawn**
38. Roger Smith, Loughborough A ReaxFF potential for radiation damage modelling of graphite
39. Roger Webb, Surrey, An Energy Deposition Profile Model for Low Energy Cluster Impacts with Molecular Solids
40. Lukasz Rzeznik, Luxembourg Numerical study on rare gas – polymer interactions on the helium ion microscope
- **41. withdrawn
42. S. Koch Karlsruhe, Development of EAM Fe-Y interaction potential towards simulation of ODS particles in iron
43. Sergey Yastrebov IOFFE, Russia, Carbon spiroids as carriers of 217.5 nm interstellar optical extinction feature
- *44. *withdrawn*
45. X. Gan, Hunan, China, The response of the Fe(001)-LI solid-liquid interface under irradiation
46. A. Rivera, UPM Simulation of intense XUV laser irradiation of band-gap materials
47. Ying Zhang Beihang, China, Molecular dynamics study of nano-scale tungsten cluster: from structure, energetics to hydrogen effects
48. Ying Zhou, Loughborough Interatomic potentials for the Ag-Ti system
49. J. Martinez-Asencio, M.J.C., Alicante IRRADIATION OF GRAPHENE: EFFECT OF INITIAL APPLIED STRAIN ON DEFECT PRODUCTION AND MECHANICAL PROPERTIES
50. Wensheng Lai *Ab initio* study of He trapping, diffusion, and clustering in Y₂O₃
- *****51. Tom Swinburne CULHAM Fast, vacancy-free climb of prismatic dislocation loops in bcc metals **Now oral**
- *****52. L. Jacques, Manchester, effects of directional electronic energy loss on simulation of radiation damage
53. M. Noble and S.P. Fitzgerald, University of Oxford and University of Leeds Modelling bubble lattices in nuclear materials
54. D. Bachurin Study of titanium beryllide for fusion applications using density functional theory methods
55. Luis Dos Santos Rosa Surrey, UK, Modelling the irradiation of a nanoporous silicon target
56. Jiechao Cui, Chengdu, Effects of surface orientation on the lifetime of near surface nanoscale helium bubbles in tungsten
- ***57. D. Danielov, Wexford, PA, USA Glancing ion beam scattering from a crystalline surface **Poster withdrawn**
58. A. De Backer H interaction with interstitial type defects predicted by MD and DFT

59. Wensheng Lai, Tsinghua, China, Vacancy enhanced mechanism for He diffusion along grain boundaries in α -Al₂O₃
60. A. Pathak, India, Positron dechannelling from stacking faults and platelets – anharmonic effects
61. C. Becquart interatomic potentials for modelling radiation damage in tungsten: A comparison with DFT

* originally Gorbunov. ** originally Bukkeroo *** poster withdrawn **** originally ranjan ***** now oral