10th International Conference on Computer Simulations of Radiation Effects in Solids

COSIRES
2010

Abstracts and Programme

Kraków, Poland
July 19-23, 2010
10th International Conference on Computer Simulation of Radiation Effects in Solids

Programme and Abstracts

Kraków, July 19–23, 2010
International Advisory Committee

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Maria Caturla (Spain)
Jean-Paul Crocombette (France)
Masao Doyama (Japan)
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Roger Webb (UK)
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Dorota Świerz

Sponsors

We would like to thank following institutions for their financial support:

Institute of Physics
The International Atomic Energy Agency
The Jagiellonian University
Prevac
# Content

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>General Information</td>
<td>7</td>
</tr>
<tr>
<td>Time Schedule</td>
<td>9</td>
</tr>
<tr>
<td>COSIRES and ICACS conference site</td>
<td>10</td>
</tr>
<tr>
<td>Programme</td>
<td>13</td>
</tr>
<tr>
<td>Abstracts</td>
<td></td>
</tr>
<tr>
<td>Oral Presentations</td>
<td>27</td>
</tr>
<tr>
<td>Poster Presentations</td>
<td>95</td>
</tr>
<tr>
<td>Author Index</td>
<td>157</td>
</tr>
</tbody>
</table>
General Information

COSIRES 2010 is the 10th International Conference on Computer Simulation of Radiation Effects in Solids. This series of conferences addresses the development and application of advanced computer modeling techniques to the study of phenomena taking place during interaction of energetic particles and clusters (from several eV to some MeV) with solids. Due to the continuous development of new theoretical methodologies and permanent increase of computer power this research field is growing fast. The application of computer simulations leads to a better understanding of basic microscopic processes taking place during and after irradiation. Fundamental understanding of such processes is often not accessible by experimental methods since they occur on very small time and length scales. However, computer simulation techniques are not only used for investigations of basic phenomena but also increasingly applied in the development of modern industrial technologies.

Conference topics include, but are not limited to:

I) Computer modeling of following phenomena:
- Sputtering
- Formation and evolution of radiation defects in materials
- Radiation responses of structural materials important for nuclear and fusion industry
- Irradiation-induced evolution of surface topography and ripple formation
- Ion beam synthesis of thin films and nanostructures
- Ion-, electron and photon-induced physical and chemical effects at surfaces, interfaces and nanostructures
- Irradiation-induced charge redistribution, electron excitation and electron-phonon interactions

II) Development of new computer modeling protocols and interatomic potentials for investigation of radiation effects.


Current meeting is organized by the Jagiellonian University in Krakow, Poland in cooperation with the International Atomic Energy Agency.
Conference Registration
Sunday, July 18, 18:00–20:00: Entrance Hall
Monday, July 19, 8:00–10:00: Entrance Hall
Conference desk will be opened from 8:30 on the other days

Conference Reception
Sunday, July 18, 19:00–21:00: Lunch area at the underground level.

Conference Venue
Auditorium Maximum of Jagiellonian University, 33 Krupnicza Street, Kraków

Lunch
Lunch area at the underground level.

Conference Outing
Wednesday, July 21, 16:15: Wieliczka Salt Mine

Conference Banquet
Wednesday, July 21, 19:00: Underground banquet chamber at the Wieliczka Salt Mine, 10 Danilowicza Street, Wieliczka

Concert
Thursday, July 22, 20:00: Large lecture hall

International Advisory Committee Meeting
Monday, July 19, 19:15: Conference room at the second floor

Accommodation
NOVOTEL CENTRUM Hotel, 5 Kościuszki Street, Kraków
OSTOYA Palace Hotel, 24 Piłsudskiego Street, Kraków
CRACOVIA Hotel, 1 Focha Street, Kraków
FORTUNA BIS Hotel, 25 Piłsudskiego Street, Kraków
LOGOS Hotel, 5 Szujskiego Street, Kraków
IBIS CENTRUM Hotel, 2 Syrokomli Street, Kraków
ALFA – Student Hotel, 17 Reymonta Street, Kraków
ALFA II - Student Hotel, 17 Reymonta Street, Kraków
ŻACZEK Student Hotel, 5 Trzeciego Maja Street, Kraków
# Time Schedule

## Sunday, July 18
- 18:00–20:00: Registration
- 19:00–21:00: Welcome Reception

## Monday, July 19
- 8:00–10:00: Registration
- 8:50 – 9:00: Conference opening
- 9:00–10:40: Session 1: Potentials and novel approaches
- 11:00–12:40: Session 2: Cluster bombardment I
- 14:25–16:05: Session 3: Cluster bombardment II
- 16:30–18:10: Session 4: Surface phenomena/Topography
- 19:15: International Advisory Committee meeting

## Tuesday, July 20
- 9:00–10:40: Session 5: Electronic stopping
- 11:00–12:40: Session 6: Emission of electrons and ions
- 14:25–16:05: Session 7: Photon/electron stimulated processes
- 16:30–17:50: Session 8: Semiconductors
- 18:00–20:00: Poster session I

## Wednesday, July 21
- 9:00–10:55: Session 9: Nanoscience (joint with ICACS24)
- 11:20–13:00: Session 10: Nanostructures
- 16:15: Conference outing to the Wieliczka Salt Mine
- 19:00: Conference dinner at the Wieliczka Salt Mine

## Thursday, July 22
- 9:00–10:40: Session 11: Materials for nuclear and fusion industry I
- 11:00–12:40: Session 12: Materials for nuclear and fusion industry II
- 14:25–16:05: Session 13: Metals and alloys I
- 16:30–17:50: Session 14: Ceramics
- 17:50–19:50: Poster session II
- 20:00: Concert at the Auditorium Maximum

## Friday, July 23
- 9:00–10:40: Session 15: Long timescale simulations
- 11:00–12:40: Session 16: Metals and alloys II
- 12:40: Closing of conference
COSIRES and ICACS conference site

Ground Floor

- Large lecture-hall
- Small lecture-hall
- Coffee
- Medium lecture-hall
- cloakroom
- Conference Office
- WC

Main entrance

Underground Level

- Lunch area
- Poster area
Programme
All activities will be held at the Collegium Maximum. Oral presentations will take place in the medium lecture hall at the ground level, except for the first session on Wednesday that will be held together with ICACS24 in the Exhibition hall at the second floor. If you intend to use conference computer, please leave the files with your presentation at the conference desk at least a day before your presentation.

Sunday, July 18

18:00–20:00   Registration
19:00–21:00   Welcome reception
<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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</thead>
<tbody>
<tr>
<td>8:00–10:00</td>
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<td>8:50–9:00</td>
<td>Conference opening</td>
</tr>
<tr>
<td>9:00</td>
<td>Session 1: Potentials and novel approaches, Chair: Kai Nordlund</td>
</tr>
</tbody>
</table>
| 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 C₆₀ Cluster Bombardment  
  *Paul E. Kennedy, Barbara J. Garrison* |
| 10:40–11:00 | Coffee break                                         |
| 11:00    | 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 CO₂ Cluster Impact on Carbon-based Surfaces  
  *Yasutaka Yamaguchi, Tomohiro Shinya, Hisato Yasumatsu* |
| 12:40–14:00 | Lunch                                               |
| 14:25    | 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 C₆₀ Bombardment of Si  
  *Kristin D. Krantzman, Barbara J. Garrison* |
| 15:25    | O10 Interaction of Energetic Clusters (Au₃, Au₄₀₀ and C₆₀) with Organic Material and  
  *Takaaki Aoki, Toshio Seki, Jiro Matsuo* |
Programme

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 SiO2
         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 Carlo Strategies
         Maurizio Dapor

12:20  O22  Molecular Ions in C60 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 Intermolecular 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 Yoshie, 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*
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>15:25</td>
<td>O42</td>
<td>Structure and Stability of $\Sigma 5$ (210) and $\Sigma 3$ (111) Grain Boundaries in Iron</td>
<td>Tomasz Ossowski, J. Kuriplach, E.E. Zhurkin, M. Hou, A. Kiejna</td>
</tr>
<tr>
<td>15:45</td>
<td>O43</td>
<td>Study of Irradiation Induced BCC Nb Precipitates in the Zr-Nb Alloy by Ab Initio Calculations and Molecular Dynamics Simulations</td>
<td>X. K. Xin, W. S. Lai</td>
</tr>
<tr>
<td>16:05–16:30</td>
<td></td>
<td>Coffee break</td>
<td></td>
</tr>
<tr>
<td>16:30</td>
<td>I11</td>
<td>Effects of Charges and Charge Transfer on Defects and Defect Generation in Ceramics</td>
<td>Fei Gao, H. Y. Xiao, W. J. Weber</td>
</tr>
<tr>
<td>17:10</td>
<td>O44</td>
<td>Calculation of Proper Vacancy Migration Energy Barriers with Artificial Neural Networks for the Modelling of Vacancy Clusters’ Migration</td>
<td>N. Castin, L. Malerba</td>
</tr>
<tr>
<td>17:30</td>
<td>O45</td>
<td>Molecular Dynamics Simulation of Threshold Displacement Energies in Lithium Aluminate</td>
<td>Hiroki Tsuchihira, Takuji Oda, Satoru Tanaka</td>
</tr>
<tr>
<td>17:50–19:50</td>
<td></td>
<td>Poster session II (even-numbered posters)</td>
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<tr>
<td>20:00</td>
<td></td>
<td>Concert at the Auditorium Maximum</td>
<td></td>
</tr>
</tbody>
</table>
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. Soulairel

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. Caturia, 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
Posters

Poster sessions will be held at the Poster area located at the underground level. All posters should be put up on Tuesday and should remain at display until Thursday evening. Odd-numbered posters should be presented by the author(s) on Tuesday, while even-numbered posters on Thursday.

**Novel approaches**

P1 Parameter Optimization in MD Simulations by Using a Genetic Algorithm
_L. Briquet, L. Angibaud, P. Philipp, J. Kieffer, T. Wirtz_

**Sputtering**

P2 Molecular Dynamics Simulation of Surface Deformation via Ga\(^+\) Ion Collision Process
_Shin-ichi Satake, Akinori Fukushige, Shun Yamashina, Masahiko Shibahara, Sadao Momota, Jun Taniguchi_

P3 Cluster Formation at Self-sputtering of Cu(001) Surface
_A. A. Dzhurakhalov, A. X. Rasulov, S. E. Rahmatov, V. G. Stelmakh, I. D. Yadgarov_

P4 Synergy in Sputtering of Copper Nanoclusters on Graphite Substrate at Low Energy Cu\(_2\) Bombardment
_G. V. Kornich, G. Betz, V. G. Kornich, V. I. Shulga, Oleksandr. A. Vromelenko_

P5 Molecular Dynamics Simulations of Low Energy Argon Ion Sputtering of Copper Clusters on Polyethylene Surfaces
_Oleksandr. A. Vromelenko, G. V. Kornich, G. Betz_

P6 Effect of Impact Angle on Sputtering of Thick Benzene by Large Ar Clusters.
_Bartłomiej Czerwinski, Łukasz Rzeznik, Robert Paruch, Barbara J. Garrison, Zbigniew Postawa_

P7 Computer Modelling of Continuous Bombardment of Ag(111) by keV C\(_{60}\) Clusters
_Robert Paruch, Łukasz Rzeznik, Bartłomiej Czerwinski, Barbara J. Garrison, Zbigniew Postawa_

P8 Stopping of Clusters in Solids
_Christian Anders, Gerolf Ziegenhain, Herbert M. Urbassek_

**Surface phenomena/topography**

P9 Topography Simulation of Sputtering Using an Algorithm with Second Order Approximation in Space
_Matthias Budil, Gerhard Hobler_

P10 Ion Milling and Ion Implantation In MBE MCT

P11 Depth Distribution of the Cobalt in Rutile (TiO\(_2\)) Implanted to High Fluences
_A. A. Achkeev, R. I. Khaibullin, L. R. Tagirov, A. Mackova, V. Hnatowicz_
Electronic stopping

P12  The Effect of Some Effective Quantities to Electronic Stopping Power
    Hasan Gümüş, Önder Kabadayi

P13  Approaches for Development of Fast Monte-Carlo Code For Calculation of The
    Electron Stopping in Substance
    V.A.Astapenko, V.V.Berezovskii, P.L.Menshikov, L.I.Menshikov

P14  Simulation of Incoherent Bremsstrahlung in Flat and Deformed Crystals
    V. V. Syshchenko, A. I. Tarnovsky, V.A. Astapenko

P15  Comparison Between Monte Carlo and Experimental Aluminium and Silicon
    Electron Energy Loss Spectra
    Maurizio Dapor, Lucia Calliari, Giorgina Scarduelli

Emission of electrons and ions

P16  Backscattered Electrons from Surface Films Deposited on Bulk Targets: a
    Comparison Between Computational and Experimental Results
    Maurizio Dapor, Nicola Bazzanella, Laura Toniutti, Antonio Miotello, Stefano
    Gialanella

P17  Kinetic Excitation of Solid Surfaces: the Influence of Projectile Impact Angle
    S. Hanke, A. Duvenbeck, B. Weidtmann, A. Wucher

Photon/electron stimulated processes

P18  Numerical Study of Formation Mechanisms of Periodic Surface Structures Induced
    on Silicon under Femtosecond Laser Irradiation
    Thibault JY. Derrien, Rémi Torres, Thierry Sarnet, Marc Sentis, Tatiana E. Itina

P19  Monte Carlo Calculation of Electron Dose Point Kernels in Water Using Different
    Transport Approximations
    Christos Bousis, Dimitris Emfietzoglou, Panagiotis Hadjidoukas, Hooshang Nikjoo,
    Anand Pathak

P20  Hybrid Continuum-atomistic Simulations for Ultrashort Pulsed Laser Ablation
    A. Maeyens, A. A. Dzhurakhalov, W. Wendelen, A. Bogaerts

Nanostructures

P21  Mechanism of Anisotropic Damage Creation Around the Track of a Sub-surface
    Channeled Ion
    Yudi Rosandi, Alex Redinger, Thomas Michely, Herbert M. Urbassek

P22  Molecular Dynamics Simulation of Nanoscale Track Formation by Swift Heavy Ions
    in Zircon
    Pedro A. F. P. Moreira, Ram Devanathan, Jianguo Yu, William J. Weber

P23  Nanocluster Modification by Swift Heavy Ion Tracks
    Olli Pakarinen, Aleksi Leino, Flyura Djurabekova, Kai Nordlund

P24  Spatio-temporal Dynamics of Ion Tracks in Silicon
    A. Akkerman, M. Murat, J. Barak
Posters

P25 Compaction and Structural Disorder Induced by Swift Heavy Ion Irradiation on Silica ($\alpha$-SiO$_2$): an MD Approach
L.P. Dávila, M.-J. Caturla

P26 Modeling Damage Accumulation in Fe and Fe-Cr Alloys Irradiated with Ions
D. Díaz, M.-J. Caturla, M. Hernández-Mayoral, M. Victoria, J. M. Perlado

P27 Simulation of End-bridge-like Radiation Defects in Carbon Multi-wall Nanotubes
A. M. Ilyin

Materials for nuclear and fusion industry

P28 First-principles Study of Point Defects and Oxygen Self-diffusion in Uranium Dioxide
Boris Dorado, Michel Freyss, Marjorie Bertolus

P29 Modelling He in Pu
M. Robinson, S. D. Kenny, R. Smith, M. T. Storr

P30 Ab-initio Modelling of W-Ta and W-V Alloys for Fusion Applications
M. Muzyk, D. Nguyen-Manh, K. J. Kurzydlowski, N. L. Baluc, S. L. Dudarev

P31 Stress Effects on Stability and Diffusion of H in Intrinsic W: a First-principles Study
Wenying Li, Ying Zhang, Hong-Bo Zhou, Shuo Jin, Guang-Hong Lu, Tianmin Wang

P32 First-principles Study of Hydrogen Behavior in V-4Ti-4Cr Alloy
Pengbo Zhang, Jijun Zhao, Ying Qin, Bin Wen

P33 Fission-fusion Mixed Neutron Field
Deng Yong-jun, Li Run-dong, LIU Yong-kang, FENG Qi-jie

P34 First-principles Investigation on the Effect of Carbon on Hydrogen Trapping in Tungsten
Shuo Jin, Yue-Lin Liu, Hong-Bo Zhou, Ying Zhang, Guang-Hong Lu

Metals and alloys

P35 Mobility of Self-interstitial Defects and Small Dislocation Loops in Fe-Cu-Ni Alloys: Model Alloy for RPV Steels
G. Bonny, D. Terentyev, V. Jansson, N. Castin

P36 The Importance of the Interaction Radius Between Cr and Self-interstitial Fe in Object Kinetic Monte Carlo Calculations of Irradiated Fe-Cr Diluted Alloys
L. Gámez, B. Gámez, M. J. Caturla, D. Terentyev, L. Malerba, J. M. Perlado

P37 Computer Simulation of Radiation Damage in Fe-Cr Alloy Produced by Neutron
W. Zhou, Y. K. Liu, D. Z. Qian

P38 Surface and Grain Boundary Segregation in Low Cr Fe-Cr Alloys: the Effect of Radiation Induced Vacancies Studied by Metropolis Monte Carlo Simulations
E. E. Zhurkin, M. Hou, J. Kuriplach, T. Ossowski, A. Kiejna
Radiation-induced Formation, Annealing and Ordering of Voids in Crystals: Theory and Experiment  
*V. I. Dubinko, A. G. Guglya*

Vacancies at Tilt Σ5 (210) and Σ3 (111) Grain Boundaries in Iron-Chromium System  
*I. Kuriplach, E. E. Zhurkin, T. Ossowski, M. Hou, A. Kiejna*

The Role of Y₂O₃ for Ods Anti-irradiation Property Revealed by Ab Initio Calculations  
*Y. D. Ou, W. S. Lai*

Nucleation and Growth of Self-interstitial Atom Clusters in β-Sic During Irradiation  
*Y. Watanabe, K. Morishita, Y. Yamamoto*

Modeling Resistivity Recovery Experiments with Event-based Monte Carlo: Beyond the Binary Collision Approximation  
*T. Luypaert, M. C. Marinica, T. Jourdan, A. Donev, V. V. Bulatov*

MD Study on Carbon Film Deposition  
*T. Muramoto, T. Hyakutake, M. Nishida, T. Kenmotsu*

Molecular Dynamics Simulations of Effects of High Electric Fields on Metal Nanotips  
*Stefan Parviainen, Flyura Djurabekova, Kai Nordlund*

Genetic Optimization of Noble Gas Clusters Doped with Metal Ions  
*Tomasz M. Gwizdała*

Free Volume Evolution in 50 MeV Li⁺³ Ion Irradiated Polymers Studied by Positron Annihilation Lifetime  
*Paramjit Singh, Rajesh Kumar, Amit Kumar, Poonam Bhatt, R. G. Sonakwade, F. Singh, D. Das, Rajendra Prasad*

Physical and Chemical Response of 145 MeV Ne⁺⁶ Ion Irradiated Polymethylmethacrylate (PMMA) Polymer  
*Rajesh Kumar, S. A. Ali, Paramjit Singh, Udayan De, H. S. Virk, F. Singh, R. G. Sonkawade, Rajendra Prasad*

Rietveld Computer Simulation of Nanostructural Perovskite Manganite by X-Ray Beam Scattering  
*G. Batdemberel, Yongfa Zhu, R. E. Dinnebier, P. Munkhbaatar, D. Sangaa, Sh. Chadraabol, T. Galbaatar*

Estimation of the Detection Efficiency for Cr-39 NTDs and the Calibration Factor for Different Dosimeter for Radon and Thoron Gas  
*Asaad H. Ismail, M. S. Jafaar*

Mass Dependence of Sputtering Characteristics for a Number of Metals with Different Properties  
*E. Yu. Zykova, A. S. Mosunov, V. E. Yurasova*
Abstracts for oral presentations
ATOMISTIC-SCALE SIMULATIONS OF CHEMICAL REACTIONS: BRIDGING FROM QUANTUM CHEMISTRY TO ENGINEERING

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Simulations have become a vital part in the understanding of chemical and physical phenomena by allowing us to gain an otherwise unattainable atomistic picture of the dynamics of these events. These simulations, however, can be both computationally and temporally intensive when considering the system size and level of accuracy we would like to achieve. Quantum calculations, for example, provide a high level of accuracy but also require a high computational cost and are limited to a relatively small number of atoms and small timescale. Conversely, empirical methods can handle much larger systems, sometimes on the order of millions of atoms, and timescales on the order of picoseconds. In order to accommodate these larger systems and timescales though, empirical methods typically employ rather simple potentials to describe the interactions of the particles with one another. Thus, there is a need to bridge the gap between these two computational realms by providing a method that retains a high level of accuracy while still modeling the interactions of atoms and molecules in a relatively simple way. This is achieved through the use of “reactive force fields”.

ReaxFF is a reactive force field technique which uses the concept of bond order to model the interactions within a chemical system. By making each interaction bond order depended, we can attain a dynamic description of each atomic and molecular interaction that does not depend on predefined reactive sites as with empirical potentials. This is done by a detailed parameterization of the atomic, bonding, angle, and torsion properties of each particle and interaction within the system, against quantum and experimental data. We are thus able to obtain a highly accurate, reactive, and dynamic model of atomic systems which can be simulated in a fraction of the time it would take to do so using quantum methods. ReaxFF also allows for the simulation of large samples on the order of thousands of particles which would be computationally impractical or impossible to simulate using quantum methods. In this presentation, we will discuss the details and development of the ReaxFF technique, as well as several applications in which it has been used to elucidate the atomic phenomena associated with radiation effects on materials.
EVALUATION OF A NEW BOND-ORDER POTENTIAL FOR Si

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The reliability and predictability of classical molecular dynamics simulations is based on the precision of the interatomic potential used. Because Si has such a great technological importance there is a clear need for more accurate potentials. Recently, a new bond-order potential has been developed [1] by modifying the well-known analytical form given by Tersoff. It has been shown that this potential can reproduce many structural and thermodynamic properties of diamond-structure Si, such as the elastic constants and the melting characteristics, and it is able to determine the cohesive energy and the lattice constants of other solid phases reasonably well [1,2]. Furthermore, the potential yields rather correct data on structure and thermodynamics of liquid and amorphous Si [2].

In the present work the new bond-order potential is applied to investigate point defect energetics and kinetics as well as solid phase epitaxial recrystallization of amorphous Si. The structure and the formation energy of the most stable configurations of vacancies and self-interstitials are determined. The migration of point defects is simulated and the characteristic migration pathways are identified. A more comprehensive study on preparation and properties of amorphous Si than in [2] is performed, and the results are compared with available experimental data. Solid phase epitaxial recrystallization is simulated at different temperatures and the recrystallization rate is determined. The results on point defect properties and solid phase epitaxial recrystallization are compared with those obtained by the Stillinger-Weber and the Tersoff potential as well as with experimental data and results of first principle calculations. Finally, a comparison is made with available results determined by two other bond-order potentials which have been recently developed [3-5].

A MODIFIED INTERATOMIC POTENTIAL FOR TUNGSTEN-HYDROGEN SYSTEM WITH DEFECTS AND THE HYDROGEN DIFFUSION BEHAVIORS

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Tungsten is one of the important candidate materials as plasma facing materials in fusion devices because it has excellent material properties such as high melting temperature, high thermal diffusivity, and low sputtering yield. However, recent experiments demonstrated that hydrogen blisters can be formed in tungsten when W is exposed to the plasma with low incident energies and high flux. The tungsten dust particles and blister exfoliations due to the break of hydrogen blisters would significantly influence the plasma performance. The hydrogen diffusivity in tungsten has a large effect on the formation of H bubbles. In this paper, we simulate the process of diffusion behaviors of hydrogen in tungsten by molecular dynamics method with a self-developed modified analytic bond-order potentials.

The interatomic potential is extremely important for the molecular dynamics simulation. Here, we construct a modified W-H and W-W analytical bond-order potentials for the W-H system. Such potentials can well repeat various properties of the W-H system from first-principles or experimental data including elastic, defect, surface and diffusion property as well as melting point. The present potential is a good choice for modelling the behaviours of H in W containing defects such as interstitial and vacancy as well as surface.

Based on such interatomic potential, the formation energy of hydrogen is calculated to be -0.22 eV and +0.21 eV for the tetrahedral interstitial site (TIS) and the octahedral interstitial site (OIS), respectively. These energies are in good agreement with those from the first-principles calculations [1]. The activation energies for hydrogen diffusing have been decided. The activation energy along the [110] direction between two neighboring TIS’s is 0.32 eV. Such activation energy is lower than the experimental value (0.39 eV) [2], but larger than that from the first principles (0.20 eV) [2]. On the other hand, the activation energy for hydrogen diffusing along [100] direction with the path of TIS-OIS-TIS is 0.65 eV, much larger than the experimental data. The diffusion behaviors of hydrogen-defect (e.g., vacancy) complexes have been also investigated.

References
MIXED RESOLUTION MODEL OF C$_{60}$ CLUSTER BOMBARDMENT

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With the emergence of cluster ion sources such as C$_{60}$, depth profiling experiments have become prominent in the field of Secondary Ion Mass Spectrometry (SIMS) [1]. In a SIMS experiment, a stream of primary ions is directed at a substrate with high energy, and upon impact of the surface, secondary molecular ions are ejected and subsequently detected. For many substrates, cluster ion sources have been shown to greatly increase the secondary ion yield in conjunction with correspondingly decreasing the surface damage to the substrate, as compared to atomic primary ion sources [1]. These features of cluster ion sources have enabled the use of SIMS to successfully depth profile through certain substrates such as the polymer poly (methyl methacrylate) (PMMA) [1, 2]. However, depth profiling through some substrates is accompanied by signal loss and remains difficult [2].

Build up of damage to the substrate in the form of carbon layers has been proposed as a primary cause of signal loss in C$_{60}$ depth profiling experiments of organic polymers [2]. Molecular dynamics simulations (MD) have been used to successfully describe physical and chemical processes that occur during energetic cluster bombardment; thus MD calculations could possibly reveal a microscopic picture of the underlying causes of the formation of carbon layers [3]. Such a MD simulation requires the use of an interaction potential that is able to describe chemical reaction. Using a reactive potential has the drawback of being computationally expensive and limits the simulations to short times or low energies [3, 4].

The goal of this work is to use the reactive force field ReaxFF to model the reactions occurring upon C$_{60}$ cluster bombardment [5]. To make such simulations computationally feasible, it is necessary to apply the ReaxFF force field only to those atoms in the system that will react. Molecules that will not undergo reactions will be coarse-grained, and their interactions with other coarse-grained particles and atoms will be calculated using a pairwise potential.

Several preliminary steps are required before C$_{60}$ cluster bombardment simulations can be started. First, ReaxFF was tested to show that ReaxFF provided acceptable reaction energetics. Second, the pairwise interaction potential between the coarse-grained particles and atoms must be optimized and tested. These two steps will be included in this presentation.

EXPERIMENTAL STUDIES OF ENERGETIC CLUSTER/SOLID INTERACTIONS – SYNERGY WITH COMPUTER SIMULATIONS

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The emergence of cluster projectiles for SIMS experiments has transformed the field over the last 5 years. These projectiles exhibit many unique properties that open a new range of experiments, particularly in molecular depth profiling and 3-dimensional imaging. Our laboratory has focused upon the use of C$_{60}^+$ due to the relatively large number of atoms in the cluster, the availability of a commercial ion source, and the possibility of focusing the beam to a submicron spot for imaging purposes. Our experiments have been intimately tied to predictions of molecular dynamics computer simulations. The nature of the C$_{60}$/solid interaction, however, introduces new complexities into how these simulations are carried out. In addition, many of the experiments that can now be performed involve distance scales and time scales that are significantly larger than those found with atomic projectiles.

In this presentation, the influence of the results of molecular dynamics calculations on our experimental program will be summarized. This influence begins with the observation that cluster bombardment with C$_{60}$ leads to significantly less chemical damage buildup than with smaller clusters such as Au$_3$. The computer simulations show that the reason for this observation is that there is much less subsurface disruption of the sample, even though both projectiles lead to the creation of impact craters. This observation was further tested using 3 nm water-ice films on Ag to show that the escape probability of the underlying Ag atoms was largest for atomic bombardment and smallest for C$_{60}$ bombardment. Computer simulations show that the mechanism of ejection involves the sweeping away of overlayer water molecules, allowing for an unimpeded escape of ejected Ag atoms [1]. These results have been critical for explaining the difference in spectra acquired using the various projectiles.

Other critical issues involve the effect of angle of incidence of the C$_{60}$ projectile on the degree of damage buildup, the maximum depth resolution achievable for buried interfaces, the mechanism of topography formation, the optimal cluster size for molecular depth profiling and the significance of the polar angle distribution of desorbed molecules. Computer simulations have been valuable at providing insight into all of these issues. Examples of how experiments using thin organic films will be utilized to show how the experiments support the predictions of these calculations.

DESORPTION OF LARGE MOLECULES WITH LIGHT-ELEMENT CLUSTERS: EFFECTS OF CLUSTER SIZE AND SUBSTRATE NATURE

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Recently, we analyzed the impacts of a series of molecular clusters on an amorphous polymeric target [1]. While the induced crater dimensions increased slightly with the projectile size (from 0.3 to 110 kDa), the sputtered mass and the number of fragments decreased drastically below a certain incident energy per nucleon. A region with significant molecular emission yield and minimal fragmentation, potentially interesting for soft desorption of organic and bio-molecules, could be identified between 0.2 and 1 eV/nucleon. Below 0.2 eV/nucleon, none of the clusters were able to desorb kilodalton molecules from the considered sample [2]. In this contribution, we focus precisely on the conditions required to desorb a large hydrocarbon molecule using carbon-based clusters. The test molecule is a 7.5 kilodalton coil of polystyrene (PS61). Several projectiles are compared, from C60 to 110 kDa organic droplets and two substrates were used, amorphous polyethylene and monocrystalline gold. The chosen hydrocarbon projectile sizes are intermediate between the polyatomic ions used in secondary ion mass spectrometry (SIMS) and the microdroplets generated, for instance, in desorption electrospray ionization (DESI). Different aiming points and incidence angles were examined. Under specific conditions, 10 keV nanodrops can desorb PS61 intact from a gold substrate (Fig. 1). However, it is more difficult with a soft polyethylene substrate. The effects of the different parameters and the underlying mechanisms are discussed, in relation with results from the recent literature [3]. The predictions of the model are also compared with results of experiments involving large noble gas and water clusters.

SENSITIVITY ANALYSIS OF CRATER FORMATION ON THE ENERGY DEPOSITION OF KEV CLUSTERS ON MOLECULAR SOLIDS

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The primary aim of the work here is to use Molecular Dynamics (MD) computer simulation to perform a sensitivity analysis of a keV fullerene impact on a molecular solid to the energy deposition process. The ultimate objective is to develop a simple model to predict the sputtering process without having to perform a MD simulation. Although MD is a widely recognized simulation technique and considered as the best means of obtaining invaluable insight into a variety of ion-solid interactions, it usually is highly time consuming. In addition, aspects such as the target size and complexity of molecular solids make the situation even more computationally taxing, thereby adding to the already lengthy simulation times. The necessity for the efforts here lies in providing SIMS (Secondary Ion Mass Spectrometry) experimentalists with an empirical software tool that can be used to optimize the choice of experimental parameters.

Previously the MEDF model of the Garrison group \cite{1} has demonstrated that the sputtering process can be well predicted by only running the first \textasciitilde100fs of an MD simulation. By analyzing how the energy has been partitioned at this time the model has convincingly demonstrated that many of the sputtering details that occur at much later times can be estimated. This still requires MD simulations to be run for a few hours/days of wall time and this simulation time is, of course, dependant on the complexity of the solid target used.

It has also been demonstrated \cite{2} that the initial impact of the cluster does not need to be simulated. By using an “Energy Dump Model” - simply allocating, an initial distribution of atoms at their initial positions, kinetic energies with values indicative of that deposited by the cluster - and then simulating using MD, the resulting craters and sputter yields are the same as that produced by running the impact. It was also demonstrated that the MEDF model could be used at the \textasciitilde100fs point to predict the final outcome in both cases.

Work presented here attempts to explore the sensitivity of this energy dump to the final outcome of aspects of the sputtering process such as crater shape and size, sputter yield and fragmentation patterns, by using which the amount of molecular ejection can be estimated. The sensitivity of this energy dump is explored by varying the dimensions of its energy density profile within the solid, benzene in the case studied here. MD simulations of course are required to be run for the varying profiles and the final prediction aims to be achieved via studies made using a reverse engineering process.


MODELING OF THERMAL SPUTTERING DUE TO CO$_2$ CLUSTER IMPACT ON CARBON-BASED SURFACES

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Previously, we have shown that the experimental sputtering yields due to size-selected (CO$_2$)$_N$ ($N=1$-$25$) impact onto a graphite surface were well reproduced by MD simulations [1]. Furthermore, the dependences of the sputtering yield on the cluster collision energy $E_{\text{col}}$ and on the parent cluster size $N$ were explained well by a thermal desorption model, where the yield was calculated from a crater surface area, a desorption barrier and an instantaneous temperature achieved by the efficient energy deposition in a local volume of the surface around the impact point.

In the present study, the modeling is extended for the impact-induced cluster ejection from various carbon-based surfaces based on MD simulations. The sputtering yields as a function of $E_{\text{col}}$ on fullerite (C$_{60}$ crystal), graphite amorphous and diamond are depicted in Fig. 1, showing that the yield increases as the target density becomes higher. Simulation results and the thermal desorption model for graphite, amorphous, and diamond are compared in Fig. 2. This indicates that the present model is applicable to targets with different densities as well.

MD SIMULATION OF HUGE REACTIVE GAS CLUSTER IMPACT WITH SUPURSONIC VELOCITY

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Cluster beams, which utilize cluster materials such as C₆₀, metal and gas clusters to irradiate on solid targets, have shown great potentials for material processing and analysis. In usual, clusters have been used as ‘ion beams’; clusters are ionized, accelerated electrically and radiated on the solid target. This cluster ion beam technique has shown higher sputtering yields with less damage to both organic and organic materials compared to conventional monomer ion beam irradiation. On the other hand, recently, it is reported that high-performance etching process are realized in specific cluster and target materials without ionization and acceleration. For example, the injection of neutral clusters consists of ClF₃ molecules, which has very high chemical reactivity to silicon, shows high-yield sputtering to silicon target (40µm/min.). Under this condition, the velocity of injected cluster is estimated as supersonic regime, which is very low compared with conventional monomer and cluster ion beam processes which has been reported previously.

In order to investigate the surface modification processes by supersonic reactive clusters, the molecular dynamics simulations of huge fluorine molecule cluster impacts on silicon targets. Figure shows the snapshot of (F₂)₁₀₀₀₀ cluster impacting silicon target with incident energy of 0.1eV/atom. As shown in the figure, the cluster does not penetrate the target surface but collapses on it. The fluorine molecules at interface between cluster and surface decompose and generates silicon-fluoride composites at very high-density. In this simulation, no silicon atoms is desorbed even 32ps after the impact, however, some silicon atoms are extracted from the surface, which are expected to leave the surface by following thermal process. In this presentation, etching processes by supersonic reactive cluster impact will be discussed from such MD simulations under various cluster size and energies.

Figure: MD snapshots of (F₂)₁₀₀₀₀ cluster accelerated with 0.1eV/atom (totally 2keV) impacting on Si(100) target.
EROSION OF Ag SURFACE BY CONTINUOUS IRRADIATION WITH SLOW, LARGE Ar CLUSTERS

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Molecular dynamics simulations are employed to probe processes taking place during continuous irradiation of Ag(111) surface by keV Ar$_{872}$ projectiles. Surface modification, the total sputtering yield, and the kinetic energy and angular distributions of ejected species are calculated at fluences ranging from 0 up to $\sim5 \times 10^{13}$ impacts/cm$^2$.

It has been shown that two trends can be identified in the development of surface roughness. At the beginning surface roughness increases fast. This fast increase terminates around $1 \times 10^{13}$ impacts/cm$^2$ and is followed by a slow increase that finally goes into saturation. The effect of the surface morphology and aggregated alteration of the bulk on the efficiency of surface erosion depends on the impact angle. At normal incidence the sputtering yield is rather insensitive to the development of the surface topography. Modification of the surface morphology has, however, a significant influence on the total sputtering yield at large impact angles. The angular spectra are always significantly influenced by the surface alteration. It is shown that bombardment events on the damaged surface exhibit a diversity of dynamics not observed on flat surfaces.
FLUENCE EFFECTS IN C_{60} BOMBARDMENT OF SI

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A recently developed simulation protocol \[1\] has been applied to model successive bombardment of Si with 20-keV C\(_{60}\) with molecular dynamics simulations. The pairing of the C\(_{60}\) projectile with the Si substrate is unique because strong covalent bonds can be formed between atoms from the projectile and substrate atoms. As a result, nearly all of the projectile atoms are incorporated into the Si lattice after impact, which results in a change in the surface composition of the substrate as a function of fluence. The results are useful in order to interpret the behavior observed in depth profiling experiments of Si with C\(_{60}^+\) cluster ion beams, in which deposits of pure carbon are developed. \[2\] With increasing projectile fluence, there is a significant transport of material both in directions perpendicular and parallel to the surface, which limits the resolution observed in depth profiling experiments. Moreover, the simulations predict a correlation between the local chemical environment of Si atoms in the substrate and the chemical composition of sputtered Si\(_x\)C\(_y\) that are formed. Therefore, the change in chemical composition in the surface as a function of fluence will alter the distribution of Si\(_x\)C\(_y\) clusters among the sputtered flux, a finding which can be compared with recent experimental data.

INTERACTION OF ENERGETIC CLUSTERS (Au₃, Au₄₀₀ AND C₆₀) WITH ORGANIC MATERIAL AND ADSORBED GOLD NANOPARTICLES

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In the last decade, the secondary ion mass spectrometry (SIMS) community has moved from atomic to polyatomic primary ions because they induce larger sputtering yields and, therefore, increase the sensitivity of the technique. Even though the underlying mechanisms are reasonably well understood today, especially for simple targets, there remain some unresolved issues. One of them concerns the interaction of cluster projectiles with hybrid metal-organic layers, such as those prepared for metal-assisted SIMS, where metallic nanoparticles condense at the surface of an organic matrix. Using molecular dynamics simulations, this contribution compares the interaction of three rather different clusters Au₃, Au₄₀₀ [1] and C₆₀, with a target of polyethylene (PE) covered by a layer of gold nanoparticles. The simulations show the differences occurring when impacts are over the Au nanoparticles or in the polymer, in terms of crater formation, yield contribution by the first layers and organic emission yield. Results show that Au₄₀₀ projectiles implant deep in the sample, producing a “suction” of the organic material, as opposed to C₆₀, which always dissipates its energy in the top layers. Au₃ induces the highest emission yields of organic material if the impacts are over the gold nanoparticle and intermediate results if the impacts are in pure PE. Lateral motion and recombination of target and projectile atoms are frequent. The observed effects are rationalized in terms of mass ratio of the projectile and sample atoms, cohesive energies of the projectile vs. impacted target and momentum of the projectiles. The results help to predict the performance of different cluster types for sputtering, as a function of the target nature.

RADIATION EFFECTS OF COPPER SINGLES CRYSTALS

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1. Outline: When a copper atom or plural atoms collide with a surface of a copper single crystal, the colliding atoms or atoms in the crystal reflect or trap in the crystal. The interactions between the colliding atoms and the surface of the crystal have been studied using computer simulations.

2. Method: Molecular dynamics have been used in the study. The atomic interactions between copper atoms are represented by an embedded atom potential determined by the authors [1].

3. Specimens: Specimens have {110}, {112}, and {111} surfaces or {100}, {110} and {110} surfaces, or a spherical shape single crystal.

4. Results: When a single copper atom hits a surface of a copper single crystal, the colliding atom is pushed back if the hitting energy is low, but if the hitting energy is large, the hitting atom enters into the crystal. An example is shown in Fig. 1. (hitting energy is 10 keV). When a single atom hits a surface of a copper single crystal with a high energy, (25 BeV, high), one atom penetrated the crystal. If hitting atom collides directly with an atom at the surface, the hitting atom is reflected even the kinetic energy is the order of 1 eV.

![Fig. 1](image1)
One Single Atom Hits the Surface With 10 keV. A Few Atoms Are Ejected.

![Fig. 2](image2)
A Cluster of Three Atoms With Energy of 1 MeV Hits (111).

![Fig. 3](image3)
A Spherical Single Crystal Specimen An atoms is hitting<111>

Figure 2 shows three atoms hitting a (111) surface of a single crystal. Some of the surface atoms are ejected. Three atom cluster hitting (111) with the energy of 10 keV/atom ejected a few atoms. Figure 3 shows one atom hitting to a spherical single crystal of <111> direction. The hitting atom entered to the specimen and another atom is pushing out from the other side. Figure 4 shows a collision of atoms on a surface, the surface atoms are ejected along a surface of a mortar. Detail discussions are given at the conference.

THE SPUTTERING CROSS-SECTION OF A SURFACE-VACANCY ISLAND

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For glancing-incidence ion bombardment, surface defects play a crucial role for controlling damage production and sputtering. In contrast to ion impact onto a flat terrace, for glancing incidence the presence of ascending surface steps, adatom islands, or a distribution of isolated adatoms, increases significantly the damage and sputtering yield. For adatom islands, the front of the defect (the ascending step edge) plays the decisive role: A violent collision between the impinging ion and the surface is activated by the front of a defect, such that the island size is a minor effect.

However, a descending step has no effect on the sputter yield. Thus, the effect of a surface vacancy island is different, since the active zone lies behind. However, while the front is inactive, it influences the ion trajectory and controls the collision of the ion with the ascending step on the tail of the defect. Using molecular-dynamics simulation we investigate the effect of vacancy islands on the creation of ion-induced surface damage. By controlling the size of the island the sputtering yield may be enhanced, but sometimes also be suppressed. This latter effect occurs, since for specific island sizes the ion deflection at the front edge prevents a violent collision of the back edge. The sputtering cross-section strongly depends on the extension of the island along the ion beam direction.
SURFACE TOPOGRAPHY INDUCED BY SWIFT ION IMPACTS

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An investigation into the development of surface topographies as a result of swift heavy ion irradiation is undertaken. It has been observed experimentally that the large amount of energy deposited in the wake of a swift heavy ion impacting the surface can have dramatic effects on the topography, with large hillocks often forming. Two models have been proposed for the formation of these hillocks and here computer simulations are carried using these models.

A thermal spike model is investigated in which atoms within a cylinder surrounding the path of the swift heavy ion are given kinetic energy due to the electronic energy loss of the projectile. In a separate model the atoms within the cylinder have their charges removed, i.e. the projectile strips the electrons from these atoms as it passes through the material. The electrons are then allowed to recombine over different timescales.

Simulations are performed in MgO with electronic energy losses comparable to those used experimentally – ranging from 15 keV/nm to 44 keV/nm. Further simulations are carried out when swift heavy ions pass through a HfO₂-MgO interface, as recent experiments have shown that craters can be produced with a raised central region.

Both models give qualitatively similar results in MgO and show the formation of hillocks on the surface above the ion track which is characterised by its much reduced density. For the case of the interface, the thermal spike model shows no crater formation but that this can occur for longer electronic recombination times in the second model. Further results will be presented at the meeting.
MOLECULAR DYNAMICS SIMULATION OF RIPPLE GROWTH IN THE PRESENCE OF Fe CONTAMINATION IN Si

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Recent experimental results [1] revealed that Fe contamination greatly affects rippling and surface morphology development in Si. This result motivated the optimization of a new parameter set for FeSi using the bond order potential (BOP) of Albe et al. The parameterization procedure has been carried out with the PONTIFIX package of P. Erhart (Darmstadt) using an extended training set of polymorph structures of FeSi (dimer, CsCl (B1), NaCl (B2), ZnS (B3), L12a (Cu3Au), L12b (Au3Cu), eps-FeSi (B20)). The energetics of various structures determined by the ab initio DFT code SIESTA. The obtained parameter set (9 independent parameters) nicely reproduce the lattice constant, cohesive energy, melting point and Bulk modulus of the most stable phase of B20 FeSi.

Recently we have shown that rippling can be simulated by classical molecular dynamics (MD) and the growth rate and the surface mean height development of preformed ripples are in reasonable agreement with experiment [2]. The new BOP potential of FeSi has been used to simulate ion induced rippling of Si with Fe contamination with classical molecular dynamics simulations (modified PARCAS code). A recently developed and lately modified c-shell script [2] is used to simulate low-energy ion-sputtering induced surface growth with Fe deposition (simulated ion-beam assisted deposition, SIBAD). The results suggest that the Fe contamination largely affects the surface properties of pure Si. Rippling can be understood as a reconstruction procedure of IBAD which is stimulated by Fe-impurities.

MODELLING HIGH THERMAL LOADS, SPATTERING AND TRITIUM RETENTION IN DIAMOND FOR FUSION APPLICATIONS

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There are many demands on the internal wall of a fusion tokamak with different areas exposed to a range of conditions. At a divertor, where waste fuel is pumped away, plasma-facing materials encounter a particularly fierce environment and need to be able to withstand high thermal shocks, chemical and physical ion erosion as well as irradiation from the high energy fusion neutrons.

Carbon has been a strong candidate in the divertor region in the form of graphite, carbon-fiber-composite materials and amorphous carbon with varying degrees of hydrogen saturation. There are, however, concerns about chemical sputtering, which will have implications for the tritium inventory. Diamond offers superior thermal and mechanical properties to other carbon materials, which may make it more suitable for the intense environment experienced by plasma-facing materials.

Understanding the dynamics of diamond under these conditions helps us understand and manipulate its strengths and weaknesses. For example, being a metastable phase, the diamond sp³ bond hybridisation will form graphitic sp² bonds if given enough energy. However, this transition may be suppressed at lower temperatures depending on lattice orientation exposed and dangling-bond passivation. The question of crystal size in a poly-crystalline surface [1] will have consequences related to tritium retention, especially at grain boundaries. Important to diamond too are the apparent effects of high temperature and hydrogen ion flux in reducing hydrocarbon sputtering yield, an important feature for concerns of plasma contamination and surface re-deposition [2]. We have used the AIREBO potential [3] to simulate high thermal loads and low energy ion bombardment in diamond. We investigate the affect of temperature and microstructure (grain boundaries and surface steps) on chemical sputtering and tritium retention.

Fig. 1. Diamond (111) surface, half is passivated with hydrogen. On heating the clean surface graphitises by 1500 K while the passivated surface remains as diamond.

BINARY COLLISION SIMULATION OF FOCUSED ION BEAM MILLING OF DEEP TRENCHES

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When a trench or hole is milled into a silicon target with a focused Ga⁺ beam, several processes take place aside from the desired sputtering: First, the target is amorphized which leads to slight swelling. Simultaneously, Ga is implanted and gives rise to a change in the sputtering yield after a few nm of the target have been removed. Later, when trench sidewalls form, they have lower Ga concentrations than the trench bottom, which again modifies the sputtering yield in addition to its angular dependence. Once the trench has reached a certain aspect ratio, the evolution of the surface topography is significantly influenced by redeposition of sputtered atoms and by backscattering of Ga ions from the sidewalls. Redeposition results in a reduced milling efficiency with increasing trench depth. Finally a stationary V-shaped trench forms, after the sidewalls have met and when the number of atoms that escape from the opening equals the number of incident ions. In this final phase ion implantation and the associated target relaxation to accommodate the added volume play important roles.

In order to simulate all these processes we have extended our previously developed code FIBSIM [1] by a target relaxation model. FIBSIM combines dynamic binary collision simulation of collision cascades with two-dimensional, cell-based topography simulation. In this approach the target is represented by the number of atoms of each species in each cell. The deviation from the ideal atomic density may be converted into a hydrostatic pressure for each cell. In the new relaxation algorithm the nodes are allowed to move in the implanted region as to minimize the strain energy associated with the pressure. Using these models we investigate the relative contributions of the above mentioned mechanisms in the different phases of trench milling. Also, we discuss limitations of the cell-based approach.

QUANTUM MECHANICAL SIMULATIONS OF ELECTRONIC STOPPING IN METALS

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During irradiation damage of metals by high energy particles, some of the incident energy is transferred irreversibly from the moving ions to the electron. Such "nonadiabatic" processes violate the Born Oppenheimer approximation, on which all classical interatomic potentials rest. By treating the electrons of a metal explicitly and quantum mechanically we are able to explore the influence of electronic excitations on the ionic motion during irradiation damage.

Simple theories suggest that moving ions should feel a damping force proportional to their velocity and directly opposed to it. In contrast, our simulations of a forced oscillating ion [1] have revealed the full complexity of this force: in reality it is anisotropic and dependent on the ion velocity and local atomic environment. A large set of collision cascade simulations [2] has allowed us to explore the form of the damping force further. We have a means of testing various schemes in the literature for incorporating such a force within molecular dynamics (MD) against our semi-classical evolution with explicitly modelled electrons. We find that a model in which the damping force is dependent upon the local electron density is superior to a simple fixed damping model. We also find that applying a lower kinetic energy cut-off for the damping force results in a worse model. A detailed examination of the nature of the forces reveals that there is much scope for further improving the electronic force models within MD.

ELECTRONIC EFFECTS IN RADIATION DAMAGE SIMULATIONS IN METALS AND INSULATORS

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Classical cascade simulations neglect the effects of the interchange of energy between the atomic nuclei and the electrons. These effects include the inelastic energy losses due to electronic stopping, energy storage and transport by the electrons and redistribution of electronic energy to the lattice. We have developed a method for including these effects in classical molecular dynamics simulations of metals.\(^1\) We couple the atomistic simulation to a coarse-grained model for the electronic energy, which evolves via the heat diffusion equation. Energy is exchanged between the atomistic simulation and the coarse-grained model at each time step. The model has been used to model low energy radiation events, swift heavy ion irradiation and sputtering events in metals. For low energy events the energy storage was found to enhance defect annealing, caused by slower cooling of the molten region. For very high energy radiation, such as swift heavy ion irradiation, energy is deposited primarily in the electronic system. This energy is transferred to the electrons via electron-phonon coupling and, above a threshold stopping power, a cylindrical molten region is formed in the crystal, which results in an elongated track of defects. Results for cascade,\(^2\) swift heavy ion\(^3\) and sputtering\(^4\) (figure 1) simulations will be presented.

The model is currently being extended to insulating materials, which are generally more susceptible to radiation damage than metals. In these materials electronic excitations create free electrons and holes, which diffuse through the material before relaxing to the ground state. During the relaxation some energy is lost to photon emission and some energy is transferred to the lattice, resulting in lattice heating. The insulator case is modelled by introducing additional transport and conservation equations for the carriers (electrons and holes). Preliminary results for the model will be presented.


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(a)  
(b)

Figure 1 The damage (vacancies, blue; interstitials, gold) created by a 5keV W atom impinging on a W surface. Figure 1a shows a conventional constant energy simulation and figure 1b shows the results from a simulations that includes electronic effects.
MOLECULAR DYNAMICS STUDY OF Si SPUTTERING AND TRACK FORMATION IN SWIFT ION INTERACTIONS WITH AMORPHOUS SiO₂

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Sputtering yields from MeV ion-matter interactions have been shown to depend on both the details of the electronic energy deposition on the lattice following ion passage, and the details of the subsequent transport. Electronic sputtering thus provides a strong, and experimentally accessible, test of fundamental processes from the femto-second to the pico-second scale. Measurements of the track structure and radius in amorphisable materials provide a similar test of the initial energy transfer to the lattice and the subsequent atomic rearrangement. Experimental results for both track radius and sputtering yield are available for a range of electronic energy loss values, and provide an opportunity to discriminate between and refine theoretical models.

In this work, we use classical molecular dynamics simulations and different models for the initial energy deposition to explore the dependence of the track radius and sputtering yield of Si from amorphous SiO₂, for different values of the electronic energy loss. The random network to describe the pristine amorphous silica sample is generated using the WWW method. The inelastic thermal spike model and a uniform cylindrical deposition of the effective energy loss are used to model the initial energy deposition. The Samela-Watanabe potential function is used for the subsequent molecular dynamics transport.

Experimental results for the variation of the track radius and sputtering yield with electronic energy loss, and also inelastic thermal spike model calculations for these quantities, are compared with simulated values using inelastic thermal spike and uniform cylindrical initial deposition models. We discuss model parameters capable of simultaneously reproducing the experimental track radius and sputtering yield across a range of electronic energy loss and projectile velocities.
SIMULATION OF SPUTTERING OF A MULTILAYER MOLECULAR SOLID BY MEV ION IMPACT

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Recent experimental work using 10MeV O$^{4+}$ ions to image fingerprints [1] via the PDMS [2] (or MeV-SIMS [3]) technique demonstrated that MeV ions can be used to image molecular ions with micron resolution. This experimental work also reported depth profiling results for both keV and MeV SIMS on samples where fingerprints had been deposited both under and over a line of ink.

The keV results of depth profiling were not surprising, as depth profiling molecular solids with high precision has been demonstrated many times in the past. However the MeV results were quite surprising as the PDMS technique using MeV ions was thought to be destructive to the molecular target. The MeV ions deposit their energy via electronic collisions rather than through nuclear collision processes. The range of the MeV ions is several 10s of microns. The energy loss process is expected to break most of the bonds in the molecular solid that the ion interacts with as it slows down. Thus it is possible to obtain a molecular image by remaining below the static limit (ensuring that ion dose is such that ions interact with less than 10% of the surface area) but once the static limit is breached the amount of intact molecular material will start to decline. The idea that it should be possible to strip away the surface layer and reveal an intact layer seems to be unlikely. However the experimental evidence seems to suggest that signals from deeper layers increase as the signals from the surface layers decrease, implying that undamaged material from deeper layers is surviving intact allowing some depth profiling information to be obtained.

We investigate here the behaviour of a simple layered molecular solid after the passage of an MeV ion has passed through it to obtain insight into how what is seen experimentally might be explained.

ION INDUCED ELECTRONIC EXCITATION OF SOLIDS: MODEL CALCULATIONS AND EXPERIMENT

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The impact of an energetic particle onto a solid surface generates atomic motion as well as electronic excitation. One of the most obvious manifestations of kinetic excitation is the fact that electrons as well as excited or ionized particles are emitted from a bombarded surface even if the projectiles carry no potential energy at all. Although being investigated for decades, the physical mechanisms behind the conversion of kinetic into electronic energy are still not completely understood. Published analytical model descriptions of inelastic processes like kinetic electron emission (KEE) or secondary ion formation are generally based on relatively coarse assumptions concerning the particle dynamics in the collision cascade initiated by the projectile impact. For instance, most KEE models restrict the excitation process to the electronic stopping of the projectile, disregarding the motion of recoils generated by nuclear stopping. Secondary ion formation models, on the other hand, often disregard the kinetic excitation process altogether and treat the solid as a quiescent electron gas interacting with a particle moving away from an idealized surface.

In principle, one would choose to describe kinetic excitation phenomena by ab-initio molecular dynamics simulations following a projectile impact. While such calculations are now possible for small systems consisting of a few atoms at small energies, they are still far too complex for the large system sizes needed to simulate a keV particle bombardment event. We therefore use a hybrid model combining classical molecular dynamics (MD) simulations with simple approximative descriptions of the electronic excitation generated by the particle motion as well as its transport away from its spot of generation. As a result, a local excitation energy density profile is calculated which can then be parametrized in form of a space and time dependent electron temperature of the solid. These data can then be employed to calculate secondary electron or ion emission characteristics for each individual projectile impact. If averaged over many events, this allows the prediction of statistical observables which can be compared with corresponding experimental data. The talk will illustrate the current state of these calculations and briefly discuss possible future developments of the technique.
MODELING KINETIC ELECTRON EMISSION WITH MOLECULAR DYNAMICS

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The electronic excitation generated in an atomic collision cascade manifests, among others, in the emission of secondary electrons. Although being investigated for several decades, the physical mechanisms behind this kinetic electron emission (KEE) process are still not completely understood. Simplified analytic models often use relatively coarse assumptions concerning the particle dynamics in the cascade and the accompanying electronic excitations. Ab-initio molecular dynamics calculations, on the other hand, inherently incorporate the electronic degree of freedom but are still hampered by the large system sizes needed to simulate particle bombardment of surfaces with keV projectile impact energies.

In order to include the microscopic particle dynamics following a projectile impact into the treatment of KEE, we use classical molecular dynamics (MD) calculations in combination with simple approximative models describing the electronic excitation generated by the particle motion. Based on a free electron gas picture, the model takes into account electronic friction experienced by all moving particles as well as electron promotion in close atomic collisions as the basic mechanisms converting kinetic energy of the particles into electronic excitation energy. The transport of excitation energy away from its spot of generation is then treated in a diffusive approach. This way, an excitation energy density profile within the cascade volume is calculated and parametrized in form of a time and space dependent electron. Using a generalized thermionic emission model, these data can then be employed to calculate KEE yields for each individual projectile impact. If averaged over many impacts, this allows to predict statistical observables which render themselves for comparison with experimental data. In this contribution, we use to model to understand the influence of projectile parameters like impact energy and angle on the KEE yields observed for metallic surfaces.
SECONDARY ELECTRON EMISSION YIELD CALCULATION PERFORMED USING TWO DIFFERENT MONTE CARLO STRATEGIES

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The secondary electron emission yield is calculated by using two different Monte Carlo strategies. The first one takes into account all the single energy losses suffered by each electron in the secondary electron cascade. It has been demonstrated to be very accurate for the calculation of the secondary electron yield and of the secondary electron energy distribution as well (see, for example, Ref. [1]).

On the other hand, since it corresponds to a very detailed description of the physical phenomena involved in the secondary electron generation process, it is relatively slow. Due to the very high number of inelastic collisions involved in the secondary electron cascade, a lot of computer time is spent in following all the particles: notice, furthermore, that many of them do not emerge from the target surface.

A faster way to calculate the secondary electron yield is based on a continuous-slowing-down approximation and uses the electron stopping power. For the use of the stopping power in the calculation of the secondary electron yield see, for example, Refs. [2-4].

According to Lin and Joy [5], the rate at which the secondary electrons are generated, as a function of depth, is given by the stopping power divided by the effective energy required to produce a secondary electron, and the secondary electron emission yield can be expressed as the integration over depth of the emission rate multiplied by the probability that a generated secondary electron is able to escape back to the surface of the target.

A Monte Carlo code based on this idea is demonstrated to be much faster than the Monte Carlo code that takes into account all the details of the inelastic collisions.

This work is aimed at comparing the yields calculated by these two Monte Carlo strategies with the available experimental data.

MOLECULAR IONS IN C\textsubscript{60} BOMBARDMENT OF SOLIDS

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Secondary ion mass spectrometry (SIMS) of organic solids is a technique that revolves around detecting the parent molecular ion, \( M^+ \), or sometimes species such as \((M+H)^+\), \((M-H)^-\) or \((M-OH)^+\). Precise measurements of these ion yields are difficult to obtain but estimates range from one parent ion per every 100 to 100,000 impacts. Recent measurements of useful yields for \( \text{Ar}^+ \) and \( \text{SF}_5^+ \) bombardment[1] are consistent with this rough estimate. These yields seem incredibly small given that simulations of C\textsubscript{60} bombardment on molecular targets show that all the energy (10-120 keV) is deposited in the top 2-3 nm of the substrate in a time of 50-100 fs.[2; 3; 4; 5] There is ample energy (or energy density) for many ionization events to occur on every C\textsubscript{60} impact, yet only a miniscule number of impacts yield molecular ions.

Molecular dynamics (MD) simulations have been used successfully to explain the motion of the atoms and molecules in cluster bombardment. Incorporation of any ionization process in the simulation is not tractable, however. First, the mechanism of ionization is not known so including a sensible model is not possible. Second, the yields are so low that the number of simulations required to observe one ionized molecule is not computationally feasible. Even though the MD simulations cannot directly model the ionization event, we propose that they give sufficient information to provide insight into the ionization mechanism. Specifically, we propose that a space-time divide exists whereby the fragment ions form in the region where the C\textsubscript{60} makes the direct impact and deposits all of its energy. The intact molecules eject from a region further from the impact region at longer times via a fluid flow mechanism. Thus, a space-time divide exists between fragment ion formation and molecule ejection. The logical conclusion is that the molecular ions are ‘preformed’ prior to ejection,[6] thus accounting for their low yield.

The proposed mechanism along with confirming experimental data by Willingham et al. [7; 8] will be discussed.

ATOMIC-LEVEL SIMULATIONS OF LASER INTERACTIONS WITH METALS: MECHANISMS OF MELTING AND RESOLIDIFICATION, GENERATION OF CRYSTAL DEFECTS

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Atomic-level computer modeling has the ability to provide detailed information on the complex processes induced by short pulse laser irradiation of metal targets and can assist in the advancement of laser-driven applications. Recent results obtained in simulations of laser interactions with metal targets [1-4] are reviewed in the presentation with a particular focus on the laser-induced generation of crystal defects and the role of the microstructure of the target on the material response to the fast laser energy deposition. In particular, to address the role of the microstructure of the irradiated target on laser-induced phase transformations, the results of the simulations of short pulse laser melting of single crystal films and bulk targets [1] are compared with computational predictions obtained for nanocrystalline Au films [3]. A description of the thermophysical properties of Au that accounts for the contribution of the thermal excitation of d-band electrons [5] is incorporated into the model and is found to play a major role in defining the kinetics of the melting process. The effect of nanocrystalline structure on the melting process is investigated for a broad range of laser fluences. At low laser fluences, close to the threshold for the complete melting of the film, the initiation of melting at grain boundaries is found to steer the melting process along the path where the melting continues below the equilibrium melting temperature of the material and the crystalline regions shrink and disappear under conditions of substantial undercooling. The unusual melting behavior of nanocrystalline films is explained based on thermodynamic analysis of the stability of small crystalline clusters surrounded by undercooled liquid [3].


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MOLECULAR DYNAMICS SIMULATIONS OF MATRIX ASSISTED LASER DESORPTION IONIZATION: ANALYSIS OF INTERMOLCULAR MATRIX-ANALYTE INTERACTIONS

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There is synergy between Matrix Assisted Laser Desorption Ionization (MALDI) experiments and Molecular Dynamics (MD) simulations. To understand analyte ejection from the matrix, MD simulations have been employed.[1; 2] Prior calculations show that the ejected analyte molecules remain solvated by the matrix molecules in the ablated plume.[3] In contrast, the experimental data shows free analyte ions.[4] Analyte molecule ejection may depend on the microscopic details of analyte incorporation in the matrix. It is important to understand the factors that influence the embedding of the analyte in the matrix and its subsequent ejection. Our calculations analyze the influencing factors such as analyte size, interaction with the matrix, nearness to the sample surface, and sample preparation.

To address the discrepancy, intermolecular matrix-analyte interactions have been studied by focusing on 2,5-dihydroxybenzoic acid (DHB), a popularly used matrix. Analytes are mainly bio-molecules which are composed of amino acids (AA). We performed MD simulations using Chemistry at HARvard Molecular Mechanics[5] (CHARMM) force field on a series of AAs to analyze the AA-DHB interaction. A relative scale of matrix-philicity/phobicity has been developed to classify AAs. Matrix-philicity/phobicity scale provides binding energy ($BE$) characteristic of AA-matrix in contrast to previous calculations that treated all AAs with one generalized $BE$. Due to structural differences in AAs, some were found to be DHB-philic ($BE \sim 34\%$ more attractive than DHB-DHB $BE$), and others to be DHB-phobic ($BE \sim 38\%$ to $\sim 70\%$ less attractive than DHB-DHB $BE$). To understand analyte release from the matrix cluster, the most phobic AA on the scale (Alanine) was studied. The results from CHARMM calculations have been incorporated in the hybrid model of bead-and-spring with breathing sphere model for performing MD simulations in MALDI. [1] We are performing MD simulations to study effect of the change in size and change in $BE$ characteristic of a particular AA on the analyte molecule ejection.

ATOMIC MIXING AND STRUCTURAL TRANSFORMATIONS IN Ag/Au FILM – Cu SUBSTRATE SYSTEMS IRRADIATED BY FEMTOSECOND LASER PULSES

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The mechanisms of femtosecond laser-induced transient melting and atomic mixing in targets composed of 30 nm Ag or Au films deposited on a bulk Cu substrate are investigated with a model combining the molecular dynamics method with a continuum description of laser excitation, electron-phonon equilibration, and electron heat conduction [1]. The initial energy redistribution and the depth of the region undergoing melting and resolidification are strongly affected by the difference in the strength of electron-phonon coupling of the film and substrate materials and by the transient variations of the electron-phonon coupling related to the thermal excitation of lower band electrons. The physical origins of the difference in the concentration profiles in the Ag-Cu and Au-Cu systems and the crystal defects generated at different laser fluences are discussed in the presentation.

Figure. The results of a simulation of laser-induced atomic mixing in a layered Cu-Ag system irradiated by a 200 fs laser pulse at a fluence of 130 mJ/cm². The concentration profile in the interfacial region is shown in (a), atomic structure of the interface is shown in (b-d), where the atoms are colored by their types in (b) and by the local structural surroundings in (c,d). Atoms with local fcc environments are blanked to expose crystal defects in (d).


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ORIENTATION DEPENDENCE OF NEAR-THRESHOLD DAMAGE 4H PRODUCTION BY ELECTRON IRRADIATION OF 4H SiC AND DIAMOND

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4H SiC Results: A wide range of epitaxial layers of electronic grade materials has been electron irradiated with electrons with energies close to the C displacement threshold (~ 95 keV) for incidence on the {0001}. Si and C faces. After irradiation the samples were studied by microscopic low temperature photoluminescence spectroscopy (PL) using 325 nm laser excitation. The spectra exhibited some of the so-called alphabet lines [1] and were dependent on the electron energy. Results will be discussed for electron energies of 120, 110 and 100 keV. 100 keV Si-face irradiation of rather pure Al- or N-doped materials (without (DAP) donor-acceptor pair emission) gave almost identical spectra with only g lines. As the electron energy was raised to 110 and 120 keV the p-doped material exhibited f-line PL while the n-doped material had e-lines. Both had b, c and d lines for these electron energies. Quite different results were obtained from the more limited range of C-face material available. These had only b lines after 100 keV irradiation and as the electron energy was raised c and d PL appeared but with lower intensities than for the same electron energies on the Si-face. Some results are shown in Fig. 1. Rather different spectra were obtained from highly doped samples, samples exhibiting DAP PL and semi-insulating samples and these will also be discussed. Although the experimental results reveal a marked asymmetry for irradiation of the different faces in other respects there is no other agreement with the many results of published molecular dynamics calculations whether based on empirical potentials (even if thermal effects are included) or on ab initio calculations. None of the optical centres that are observed involve either dumb-bell configurations of C-interstitials or Frenkel pairs. The available evidence indicates that the observed PL originates from centres involving anti-sites, either antisite pairs or C-antisite-C-vacancy pairs. It will be argued that future calculations need to take account of the energy provided by electron and hole recombination after their creation during irradiation. The experimental evidence that leads to this conclusion will be presented.

Diamond Results: very pure diamond samples have been electron-irradiated along [100], [110] and [111] to investigate the decrease in vacancy production as the displacement threshold is approached from above. The results have been analysed in terms of the McKinley-Feshbach asymptotic approximation of the Mott cross-section (see Fig.2).

DIFFUSION PHENOMENA IN ISOTOPOICALLY CONTROLLED SEMICONDUCTOR HETEROSTRUCTURES

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Isotopically controlled semiconductor heterostructures of silicon (Si) and germanium (Ge) are very advantageous for self- and dopant diffusion experiments. By means of such structures the impact of dopant diffusion on self-diffusion can be investigated which provides valuable information about the mechanisms of atomic diffusion and the charge states of the point defects involved. The usefulness of simultaneous self- and dopant diffusion experiments is first demonstrated by dopant diffusion in Si isotope multilayer structures [1]. The results of this study are compared to conventional diffusion experiments that consider self- and dopant diffusion separately.

Presently the elemental semiconductor Ge has received renewed interest due to its potential use in the fabrication of complementary metal oxide semiconductors. By utilizing Ge instead of Si one can take advantage of the higher electron and hole mobilities in Ge compared to Si. For the fabrication of Ge-based electronic devices the diffusion and activation of dopants must be controlled. This requires an in-depth understanding on the mechanisms of dopant diffusion and on the type of the native point defects involved. In this talk experiments on the diffusion of donor and acceptor dopants in natural bulk Ge and isotopically controlled Ge multilayer structures are presented. Analysis of the experimental profiles shows that doubly negatively charged vacancies mainly determine self- and dopant diffusion under intrinsic and n-type doping conditions [2,3]. No evidence of Ge interstitials in self- and dopant diffusion is found. However, the diffusion behaviour in Ge changes considerably under in situ proton irradiation. Self- and dopant diffusion in Ge under proton irradiation reveals that self-interstitials dominate the diffusion process under irradiation [4]. The origin of this unexpected behaviour and emerging new strategies for the fabrication of Ge-based nanoelectronic devices are discussed.

OPTIMIZATION OF AMORPHOUS SILICON AND SILICA STRUCTURES FOR MOLECULAR DYNAMICS SIMULATIONS

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Quality of amorphous structures used in molecular dynamics simulations is a critical factor to reliable results. For example, nanopattern formation on silicon surfaces under ion beam radiation is a coherent effect of small displacements induced by individual impacts. To detect these displacements the amorphous structure should be free of internal stresses and its density should correspond the density of the real material.

The WWW algorithm [1] is considered one of the best optimization methods to create high-quality amorphous structures for simulations. However, it is not possible to fully optimize structures that are large enough for impact simulations. Structures of only a few thousand atoms can be fully optimized.

We have developed a practical method to create large partly optimized amorphous silicon and silica structures that give satisfactory results in impact simulations. We use first the WWW algorithm to optimize several nanometer wide amorphous structures. The optimization is done in parallel computing environment. Then we use these small structures as building blocks of larger structures. Finally, the structure is further relaxed using the particular interatomic potential applied in the impact simulations.

The density and characteristics of these amorphous structures correspond very well the properties of real structures. The majority of the Si atoms are four-fold coordinated. The amorphous networks are free of internal stresses which makes it possible to detect weak displacement fields induced by 100 eV Ar atom impacts, for example. In the paper we discuss the application of the structures on model development of nanopattern formation.

The optimization process developed opens a possibility to simulate also large-scale cluster ion impacts on silica.

LOW-ENERGY OXYGEN BOMBARDMENT OF SILICON BY MD SIMULATIONS MAKING USE OF A REACTIVE FORCE FIELD

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In the field of Secondary Ion Mass Spectrometry (SIMS), ion-matter interactions have been largely investigated by numerical simulations. For MD simulations related to inorganic samples, mostly classical force fields assuming stable bonding structure have been used.

In materials science, level-three force fields capable of simulating the breaking and formation of chemical bonds have recently been conceived. One such force field has been developed by John Kieffer[1-5]. This potential includes directional covalent bonds, Coulomb and dipolar interaction terms, dispersion terms, etc. Important features of this force field for simulating systems that undergo significant structural reorganization are (i) the ability to account for the redistribution of electron density upon ionization, formation, or breaking of bonds, through a charge transfer term, and (ii) the fact that the angular constraints dynamically adjust when a change in the coordination number of an atom occurs.

In this work, we will present results obtained for the simulation of low-energy oxygen bombardment of silicon. Variations of sputtering yields and angular distributions will be studied in particular. Compared to normal force fields, ion-matter interactions as well as the sputtering of matter should be described more accurately, especially when using reactive primary ions (oxygen or cesium) at low impact energies. The simulation results will be validated by comparison to experiments.

INTERACTION OF CHARGED PARTICLES WITH INSULATORS AND LIVING CELLS

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This tutorial talk consists of two recent topics concerning charged particle interactions with matter, (1) the interaction of slow highly-charged ions with insulators, where a self-organized charge up process often plays the key role in inducing various interesting phenomena such as a guiding effect [1], and (2) the micro-beam generation [2] of MeV ions by a tapered glass capillary with a thin cap, which for the first time enables micro-irradiation of living cells [3] as well as micro-modifications of liquid-solid interfaces [4].

The guiding effect has been studied intensively for insulator foils with many straight and parallel nano-holes (multi-microcapillary). It was found e.g., highly charged ions transmit along the microcapillary keeping their charge states even when the microcapillary is tilted against the beam direction. In this case, the incident beam deposits charges on the inner-wall of the capillary, and induces a repulsive force on the incoming charged particles, which eventually guides the incident beam to the direction of the capillary. Actually, it takes some macroscopic time for the beam to stably transmit, where deposited charge governs the phenomena. Such a guiding effect was also observed for a single tapered glass capillary accompanied by a beam density enhancement (focusing effect). In other words, a tapered glass capillary provides a new scheme for the generation of a microbeam of highly charged ions, which is otherwise quite difficult if not impossible.

Meanwhile, a similar focusing effect was also found for MeV ions transmitted through a tapered glass tube. In this case, the beam transmission takes place immediately after the beam injection without time delay, i.e., the primary transmission mechanism is not a charge up but a result of successive multiple small-angle scatterings. In this sense, the MeV ion guiding is not very interesting as physics, but instead this enables for the first time a pinpoint bombardment of a μm³ volume in an arbitrary position in air and in liquid without affecting accelerator vacuum if a thin cap is prepared at the tip of the capillary. Various applications to high-resolution 3D mapping via micro-PIXE, -RBS, and resonant nuclear reaction have already been studied, one of the potential application is a so-called cell surgery where a specified organelle of a living cell at the specific cell cycle is bombarded to search for differential radiation effects [6].

ION BEAM MODIFICATION OF NANOCRYSTALS: SIMULATION AND EXPERIMENT

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Ion beams of a broad range of energies are widely applied to modify the properties of materials. The nanotechnology, intensively developing over the last decades, has given rise to a clear urge for the possibility of controllable modification of the properties of structures comprising nanoparticles. The application of ion beams for this purpose is seemingly very appropriate. However, thanks to the limited size of nanoparticles (from a few to 10s of nm), the response of the structure modification can be surprisingly different from the one, expected from their bulk counterpart.

The attention of the scientific community has been drawn to the ion modification of the nanoparticles since the beginning of 1990s (Fig.1), and many interesting findings and observations have been reported. The focus here will be to overview the experimental observations and computer simulations of the sputtering and structural modification of nanocrystals (NCs) in free-standing and embedded NCs under ion and swift heavy ion irradiation.

Free-standing NCs (or ones weakly interacting with a substrate) are an ideal system for scientific study as single NCs can be characterized by e.g. TEM and modified by ion beams without any effects from the surrounding. For instance, metal NCs deposited on organic substrates have been shown to enable secondary ion mass spectrometry (SIMS) analysis of very large organic molecules [1], or light ions have been shown to be able to transform polycrystalline nanoparticles into single crystal ones [2].

For nanocrystals embedded in solids, energetic ions offer several interesting possibilities for cluster processing that cannot be achieved by any other means. Ion beam processing of existing nanocrystals can be used to introduce defects into them, beneficial for optical properties. Even more surprisingly, it has recently been shown that swift heavy ions can be used to generate elongated nanocrystals with aspect ratios up to 100, changing the dimensionality of the nanoobject from a 0D nanocrystal to a 1D nanorod. The talk will also present our recent work on modelling of ion irradiation of both free-standing and embedded NCs.


THRESHOLD DEFECT PRODUCTION IN MECHANICALLY STRAINED SINGLE-WALLED CARBON NANOTUBE AND SILICON NANOWIRE

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The intriguing behavior of nanomaterials subjected to electron and ion irradiation has stimulated a large body of experimental and theoretical work aimed at understanding irradiation effects in nano-scale systems and at using particle beams as a tool to tailor their properties\cite{1}. In all previous experimental studies the irradiation was carried out first, and then the mechanical properties of the system were determined. However, the question of how mechanically strained nanomaterials respond to ion or electron bombardment has never been addressed.

This question is not only of fundamental but also of high practical importance, as the radiation hardness of various nanostructures may deteriorate significantly as a function of mechanical strain, especially when the strain approaches the elastic limit. Two systems representative of such strained nanostructures subjected to irradiation are single-walled carbon nanotubes (SWCNT) and silicon nanowires (Si NW), the former as found in e.g. the long discussed space elevator and the latter in any sensor or solar cell application in space.

Using a density-functional theory based method and classical molecular dynamics simulations, we have studied the response of mechanically strained SWCNT and Si NW to electron irradiation. It is found that the threshold displacement energy for a carbon atom in the wall of a nanotube depends strongly on the strain and the tube chirality, showing a drop in the displacement energy of about 10% for strains of 10%. For the Si NW, we find that the sputtering threshold energy stays nearly constant, but the threshold displacement energy in the bulk core of the wire depends heavily on the mechanical strain. The threshold energy averaged over all lattice directions decreases by 30% for a strain of 10%. Additionally, we find that the threshold energies are correlated to the formation energies of the relevant point defects.

THE EFFECT OF HELIUM BUBBLE ON THE MECHANICAL PROPERTIES OF PALLADIUM NANOWIRE

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This paper presents the effects of helium bubble on the mechanical properties of palladium nanowire, under the continuous tensile strain at 300 K by molecular dynamic simulations. Our result shows that the presence of helium bubble facilitates the rupture of nanowire and reduces its ductility. Also, the rupture strain decreases with the increase of helium bubble’ size. It is found that the nanowire cracks around the bubble due to its obvious inhibition for the relative glide of planes. The inhibition is determined by the size of helium bubble. As the diameter of bubble exceeds ~1.2 nm, the nanowire’s phase transformation and relative glide are inhibited clearly, which is defined as critical size of bubble. It is shown that the glide planes cannot completely cross over the bubble while it exceeds the critical size.
MECHANISM OF SELECTIVE NANO STRUCTURE FORMATION ON PRE-PATTERNED SURFACES

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During oblique metal vapor deposition perpendicular to ripples of pre-patterned surfaces, a chain-like formation of metal nano clusters along the ripples has been observed. The metal nano clusters are located on the slopes which point towards the evaporation source. The self-ordering of metal nano structure formation has not been observed for normal deposition and for low-angle deposition parallel to the ripple direction. The features of the metal nanostructure depend on the evaporation angle and surface morphology of substrates. With the 3D lattice kinetic Monte Carlo simulations we studied the process of silver deposition on pre-patterned, oxidized Si surfaces. The experimentally observed Ag nano structures were reproduced. It was shown that the extremely short range of surface adatom migration together with a slope-dependent deposition rate promotes the two dimensional local Ostwald ripening and consequently, strongly selective Ag nanocluster nucleation appeared on the high deposition spot of surfaces.
STRUCTURE OF SI/GE NANOCLUSTERS AS STUDIED BY MOLECULAR DYNAMICS AND SEMI-GRAND-CANONICAL MONTE CARLO METHODS

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Ionized cluster beam deposition can be used to create anything from individual nanostructures to nanocrystalline films, depending on the amount of clusters deposited and the deposition energy. Experimentally, there is a number of ways to make these atomic clusters – for example, the newly constructed facility at the University of Helsinki Department of Physics employs a magnetron sputtering device and a condensation chamber filled with argon to condense the clusters. The clusters thus formed can then be accelerated and deposited onto the desired surface.

We have previously used molecular dynamics (MD) simulations to simulate the formation of silicon, germanium, and Si/Ge nanoclusters in an argon atmosphere at room temperature [1]. The results indicated that in the time frame of MD simulations, not all clusters were able to form radially symmetrical shapes. Whether this was an effect of short simulation time (of the order of nanoseconds), or if the resulting shapes were indeed stable, was left an open issue. In addition, it was noted that germanium atoms had the tendency to segregate to the outer layers of the clusters, which confirmed earlier findings done in our group [2].

This work continues the investigation into the energetically favorable shape and element distribution of Si and Ge nanoclusters. In addition to annealing the least spherical of the clusters to prompt radial symmetry, we use a new method that combines molecular dynamics with a semi-grand-canonical Monte Carlo algorithm to investigate the element distribution that is most favorable in terms of free energy. The results show that when annealed for at least 100 ns at 1800 K, the clusters become more spherical, and that the preferred location of the Ge atoms is indeed closer to the surface.

NANOSCALE PHASE TRANSITIONS WITHIN SWIFT-HEAVY ION TRACKS IN PYROCHLORE STRUCTURES

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The dynamics of track development due to the passage of swift-heavy ions through solids is a long-standing issue relevant to nuclear materials, age-dating of minerals, space exploration, and nanoscale fabrication of novel devices. We have integrated computer simulation and experimental approaches to investigate nanoscale phase transitions under the extreme conditions created within single tracks of swift-heavy ions in Gd\textsubscript{2}Zr\textsubscript{2-x}Ti\textsubscript{x}O\textsubscript{7} pyrochlores. Track size and internal structure depend on energy-density deposition, irradiation temperature, and material composition. Based on the inelastic thermal spike model, molecular dynamics simulations follow the time evolution of individual tracks and reveal the phase transition pathways to the concentric track structures. For Gd\textsubscript{2}Ti\textsubscript{2}O\textsubscript{7}, the track core is amorphous and surrounded by a defect-fluorite structure, with an outer most structure that is highly defective pyrochlore, similar to structures observed by high-resolution transmission electron microscopy (HRTEM) \cite{1}, as shown in Fig. 1. For the intermediate composition (x=1.0), the amorphous core has decreased in radius, and the relative thickness of the defective crystalline shells has increased. In the case of Gd\textsubscript{2}Zr\textsubscript{2}O\textsubscript{7}, the core does not become amorphous, but has the defect-fluorite structure, which is also observed by HRTEM \cite{1}. The molecular dynamics simulations demonstrate that track structure depends on complex competition among melting, disordering and recrystallization processes.

\cite{1} M. Lang, J. Lian, J. Zhang, F. Zhang, W. J. Weber, C. Trautmann, R. C. Ewing, Single-Ion Tracks in Gd\textsubscript{2}Zr\textsubscript{2-x}Ti\textsubscript{x}O\textsubscript{7} Pyrochlores Irradiated with Swift Heavy Ions, Phys. Rev. B: Condens. Matter Mater. Phys. 79 (2009) 224105.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{Fig1.png}
\caption{Swift-heavy ion tracks in Gd\textsubscript{2}Ti\textsubscript{2}O\textsubscript{7}: (a) HRTEM image \cite{1} and (b) thermal spike simulation.}
\end{figure}
MULTISCALE VIEWPOINT OF RADIATION DAMAGE PROCESS IN FUSION MATERIALS

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Component materials of a nuclear fusion reactor as an attractive future energy source, such as the first-wall structural materials and divertor materials, are exposed to the bombardment of energetic plasma-particles and neutrons, which may cause various changes in material’s microstructure and mechanical property. These are, in many cases, undesirable damage for reactors. Knowledge on material’s response to fusion irradiation is required for reactor materials design, but it should be obtained using alternative existing irradiation facilities such as nuclear fission reactors and ion accelerators, because there are no actual fusion devices at present. A precise understanding of radiation damage processes is required to achieve the reliable materials design on a basis of accurate understanding of the difference of irradiation conditions between the alternative environment and the actual environment, which is, for example, a difference in displacement damage rate (dpa/s).

Radiation damage processes occurred in materials during irradiation are, in essence, the multiscale phenomena, and a physical description of the processes involves a wide variety of physics processes, i.e., athermal ballistic binary collisions between the irradiating projectiles and lattice atoms in the initial stage, the collective motion and energy dissipation among lattice atoms in the subsequent thermal spike stage, followed by the stage of thermal activation process including defect cluster formation in materials. To model these complicated processes, multiple evaluation methods are needed to investigate them at the individual time and length scales. Also, bridging the information of different scales thus individually obtained is important to understand the entire processes.

In this paper, the Monte-Carlo simulations and the rate theory equation calculations are compared from the viewpoint of multiscale modeling, and the Monte-Carlo technique is employed to investigate the nucleation and growth process of defect clusters in materials during irradiation, where the behavior of defect cluster embryos is accurately treated by considering the stochastic fluctuation of defect flux in materials. Our results show void nucleation rates in pure metals as a function of temperature and damage rate, helium effects on void thermal stability in pure metals, the dependence of vacancy composition on void nucleation in a binary compound SiC material, and so on. All of these are very important to obtain a precise description of radiation damage processes.
HE BUBBLES GROWTH MECHANISM IN FeCr

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A detailed understanding of the thermodynamic aspects of Cr and He segregation is required to develop the capability of designing swelling resistant microstructures. We have developed a formulation of an empirical interatomic potential that incorporates the complexities of the thermodynamics of the FeCr system, adding He as a third element in the alloy, using results for Fe-He and Cr-He interactions developed by K. Nordlund’s group. We use a novel numerical approach based on variance-constrained transmutation ensemble implemented in a massively parallel hybrid Molecular Dynamics/Metropolis Monte Carlo code to study precipitation of He and Cr in grain boundaries and segregation at surfaces as a function of Cr composition. We present preliminary results on FeCr swelling under Helium irradiation and the mechanism of growth by emission of interstitial dislocation loops. Our work represents our first step in the development of modeling capabilities to describe Cr and He segregation kinetic effects induced by radiation.
TOWARDS SUPPRESSING BLISTERING BY INVESTIGATING PHYSICAL ORIGIN OF HYDROGEN/HELIUM INTERACTIONS WITH TUNGSTEN

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W is considered to be one of promising candidates for a plasma facing material (PFM) in a fusion Tokamak. However, as the PFM, W will be exposed to extremely high fluxes of H isotope ions and He, leading to surface blistering. The blistering behavior of W under H and He irradiation is one of the key concerns for the W-PFM and thus has been under intensive investigations. In order to find an effective way to suppress retention and blistering of H/He in W, we systematically investigate the H/He interaction with W using a first-principles method.

Individual H atom energetically prefers to occupy the tetrahedral interstitial site (TIS) in the bulk W, and two H in the TIS’s form a pairing cluster along the <110> directions with the H-H distance of \( \sim 2.22 \, \text{Å} \) with a very weak attractive interaction \([1]\). This suggests that H itself is not capable of trapping other H atoms to form a \( \text{H}_2 \) molecule, following which we reveal a microscopic vacancy trapping mechanism for H bubble formation in W. Vacancy provides an isosurface of optimal charge density that H prefers to stay (0.11 electron/Å\(^3\)), inducing collective H binding on its internal surface. A monovacancy can hold as many as 10 H atoms, for which a \( \text{H}_2 \) molecule forms at the vacancy center \([2]\). This will be a prerequisite for preliminary nucleation of \( \text{H}_2 \) bubble inside the vacancy. \( \text{H}_2 \) molecule and thus \( \text{H}_2 \) bubble is calculated to be not capable of forming at a W grain boundary without vacancy because of limited isosurface of optimal charge density for H \([3]\).

He prefers to occupy the lowest charge density region due to its close-shell structure. It exhibits a strong attraction with H in W and thus can be a trapping center for H, resulting from a local optimal charge density reducement due to a lattice expansion by the presence of TIS He. He-vacancy complex provides a larger isosurface of optimal charge density than that via a monovacancy without He, and thus can hold 12 H atom (Fig. 1). Importantly, \( \text{H}_2 \) cannot be formed due to the occupancy of He at the vacancy center, in consistence with the recent experiments \([4]\). The results pave a theoretical way to suppress the retention and blistering of H by changing local charge density in W, making it not ‘optimal’ for H. For example, it can be predicted that the inert gas can be doped in W to effectively suppress the H blistering.

References

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

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In order to contribute to understanding of the evolution of W microstructure in the conditions of the International Thermonuclear Experimental Reactor as well as the DEMOnstration Power Plan we parameterised our object Kinetic Monte Carlo code named LAKIMOCA. Ab initio calculations have been realized to model the behaviour of interstitial, vacancy and helium clusters diffusing in tungsten. The slowing down of atomic helium and the associated damage is determined using the Marlowe code adapted to take into account the polycrystal nature of W.

Parametrisation has been tested comparing LAKIMOCA and Soltan’s experiment [1] of isochronal annealing of W slabs irradiated by 400 eV and 3 keV He.

As illustration of the good agreement between experimental and simulated results, Figure 1 represents total number of defects and He in function of temperature for the 3 keV He irradiation of W slab.

Moreover, simulations showcase that He desorption results from a competition between the formation of mobile clusters and sessile ones. Comparaisons have been done to study the relevance of taking into account the crystal structure of W and we found that polycrystallin nature give the best agrement. It is thus very important to model correctly the damage, its spatial distribution as well as the defect and He clusters properties.


Figure 1 Comparaison of experimental and simulated number of He and defects (normalized) in function of temperature during isochronal annealing of W slab irradiated with 400 eV He
IAEA ACTIVITIES ON R&D OF STRUCTURAL MATERIALS FOR ADVANCED REACTOR SYSTEMS

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Materials performance and reliability are key issues for the safety and competitiveness of future nuclear installations being developed for sustainable nuclear energy, e.g. Gen-IV/INPRO fission reactors, fusion reactors, waste transmutation systems and fusion-fission hybrid reactors. These advanced systems will feature high thermal operating efficiencies, a maximised utilization of fuel and a minimal production of nuclear waste. The chain of challenges on basic development, qualification and deployment of new structural materials with improved mechanical, physical and radiation-resistant properties has to be addressed and solved. To achieve the required materials performance parameters, focused research and targeted testing of candidate materials is necessary. The design and engineering of such materials is increasingly being supported by theoretical calculations and computer simulations. This approach is considered to be of high importance in radiation materials science as the cost and time involved with high dose neutron irradiation experiments is prohibitive. Predictive computer modelling, backed up by experimental validation and benchmarking, is the principal motivation for developing a multi-scale approach to predict the performance of materials under high damages and long irradiation times.

Recently, there have been promising developments in new classes of advanced materials such as fibre-reinforced ceramic composites, oxide-dispersed strengthened alloys with nano-structured features and advanced reduced activation ferritic-martensitic steels. There is a strong need and demand for intensified experimental support, especially for material behaviour under extreme conditions of high dose and/or temperature. This is partially being provided by charged particle irradiation experiments, computer modelling and advanced materials characterisation techniques however, it only part of the many different activities required to provide reliable and validated data and information leading to the qualification and licensing of materials to be used in future nuclear installations.

Success will require long-term intensive and internationally collaborative and coordinated programmes of research and development and in which the IAEA can play an important role in supporting, facilitating and coordinating efforts between Member States. This paper summarises the IAEA programmatic activities on the R&D support programmes on structural materials development for advanced reactor systems and gives some outlook and future perspectives.

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RADIOPARAGENESIS: THE EFFECTS OF TRANSMUTATION ON CRYSTALLINE STABILITY

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Although public support for the expansion of nuclear power is growing, significant growth is liable to be hindered or even halted by the seemingly intractable nuclear waste problem. A particularly difficult component of the waste problem is that any solution must be highly predictable at time scales not conducive to direct experimental verification. However, we have recently discovered a phenomenon that may permit improved predictability of long-term waste form performance. Specifically, from first principles theoretical methods, we have found that unconventional compounds and crystal structures may form via the chemical transmutation that occurs during radioactive decay (e.g. rocksalt $^{137}\text{BaCl}$ formation from the $\beta^-$ decay of $^{137}\text{CsCl}$). We refer to this phenomenon as “radioparagenesis.”

At COSIRES 2008, we presented initial results on the effects of radioparagenesis in CsBaCl. In this talk, we expand on those initial findings, focusing on two aspects. First, we explore the concept of applying radioparagenesis to the evaluation of long time scale crystalline nuclear waste form performance as well as to the design of chemically robust waste forms, emphasizing the thermodynamic and mechanical stability of radioparagenetic phases. Second, we discuss the implications of radioparagenesis for the possible fabrication of novel materials, removed from waste form applications. We also propose a modification of Kröger-Vink notation to account for daughter products.


MOLECULAR DYNAMICS STUDY OF DAMAGE PRODUCTION IN URANIUM DIOXIDE UNDER IRRADIATION

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The nature of primary damage induced within a uranium dioxide matrix subjected to a flux of energetic particles was investigated using classical molecular dynamics simulations. UO2 was modeled using the set of empirical potentials described in [1], based on a rigid ion model. Displacement cascades were initiated by accelerating a uranium primary knock-on atom to a kinetic energy ranging from 1 to 80 keV between 300 K and 1800 K. Cascades were also purposely overlapped within the same simulation box so as to study the response of the material to increasing damage levels. During the cascade overlap sequence, the average density of defects within the damaged volume increases and levels off. Higher damage levels are reached when the temperature decreases. At low temperature (700 K), a distribution of nanometric cavities is directly generated through radiation effects only.

These results, in conjunction with several other observations taken from the literature of ion implanted [2] or neutron irradiated uranium dioxide, suggest a radiation damage controlled heterogeneous mechanism for insoluble fission product segregation in UO2. Interstitial dislocation loops are also formed by a loop punching process at the interface between the highly pressurized molten core of the cascade and the solid matrix. High temperatures appear to be favorable to the formation of dislocation loops and less favorable to vacancy clustering.

INTERACTION OF CARBON WITH POINT DEFECT CLUSTERS IN \(\alpha\)-Fe: AN MD STUDY

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This work deals with the characterisation of point defects such as self interstitial atom (SIA) and vacancy clusters in \(\alpha\)-Fe using molecular statics simulations.

The interaction energy of a carbon atom (in an octahedral position) with a \(1/2<111>\) 7-SIA cluster was calculated with three different inter-atomic potentials for Fe-C systems (derived by Hepburn[1], Raulot[2] and Johnson[3]). The interaction energy was calculated for every octahedral position in the habit plane (i.e. \((111)\)) of the 7-SIA cluster and the corresponding interaction energy maps were constructed. The results show that the C atom has the highest binding energy (of 0.47 eV for Hepburn, 0.39 eV for Raulot and 0.42 eV for Johnson) with the cluster, when placed just outside the edge of the cluster. All applied potentials provide qualitatively the same result.

The most energetically favourable configurations for vacancy-carbon (v\(_n\)-C) complexes of size \(n = 1 – 6\) were obtained with the above mentioned potentials. The binding energies and dissociation energies were calculated. For the Hepburn potential, the C atom was repelled by vacancy clusters of size 5 and 6 and also the formation of a v\(_2\)-C complex by coalescence of vacancy and C-v was found to be unfavourable. The opposite result was found using Raulot's and Johnson's potentials.

The most favourable vacancy-di-carbon (v-C\(_2\)) complex were obtained with the same potentials when the vacancy was placed between two octahedral C atoms. The dissociation energy for C leaving the v-C\(_2\) complex was thus 1.06 eV for Hepburn, 1.14 eV for Raulot and 1.36 eV for Johnson, whereas experiments suggest a value of 1.1 eV.

MULTI-SCALE MODELING OF IRRADIATION EFFECTS IN SPALLATION NEUTRON SOURCE MATERIALS

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Spallation neutron source is a coupling of a target and a proton accelerator. High energy protons of GeV order irradiated in the target produce a large number of neutrons. The beam window and the target materials thus subjected to a very high irradiation load by source protons and spallation neutrons generated inside the target. At present, there are no materials that enable the window to be operational for the desired period of time without deterioration of mechanical properties.

Irradiation experiments are essential for the development of such structural materials. However, there are several cases in which, materials are developed without appropriate irradiation facilities, such as fusion reactor materials. Recently, strong spallation neutron sources, SNS in the United States and J-PARC in Japan have been completed. These facilities, however, are not designed for materials irradiation experiments. Computer simulations play an important role in predicting materials behavior.

In this paper, mechanical property changes of nickel by 3 GeV protons are calculated by multi-scale modeling of irradiation effects. Nickel is considered to be a most simple model material of austenitic stainless steels. The code consists of four parts. First part is for nuclear reaction. It calculates the interaction between high energy protons and nuclei in the target based on PHITS code from 10^{-22} s. Second part is for atomic collision by particles which do not cause nuclear reactions. As the energy of particles is high, binary collision approximation is employed for the subcascade formation. In each subcascade, the direct formation of clusters and the number of mobile defects are estimated by using molecular dynamics. Third part is the formation and development of point defect clusters with freely migrating defects, which starts from 10^{-12} s. The kinetic Monte-Carlo simulation and the reaction kinetic analysis are used. The development of damage structures changes the mechanical properties of target materials. Fourth part is the estimation of mechanical property changes by using discrete dislocation dynamics. Stress-strain curves of high energy proton irradiated nickel are obtained.
MULTI-TIME SCALE MODELING OF RADIATION DAMAGE AT GRAIN BOUNDARIES

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We have used three atomistic modeling methods that span different time scales -- molecular dynamics, temperature accelerated dynamics, and molecular statics -- to investigate radiation-induced damage production and subsequent defect annealing near tilt grain boundaries in copper. The short-time (picoseconds) defect production is modeled by molecular dynamics simulations, and the resulting damaged structures are used as the input for long-time defect annealing studies via temperature accelerated dynamics simulations. Molecular statics calculations are used for calculating the thermodynamic properties of defects. We find that grain boundaries have a surprising “loading-unloading” effect [1]. In the defect production stage, interstitials are loaded into the grain boundaries while vacancies remain trapped in the bulk. In the defect annealing stage, interstitials are unloaded from the grain boundaries and emitted back to the bulk to annihilate vacancies with relatively low barriers compared to conventional vacancy diffusion. The combination of this newly found interstitial emission mechanism and conventional vacancy diffusion help explain the different radiation tolerance of nanocrystalline and polycrystalline materials under different conditions.

MICROSTRUCTURE EVOLUTION OF IRRADIATED FE IN THE PRESENCE OF HE STUDIED BY KINETIC MONTE CARLO

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It is well known that He can stabilize clusters of vacancies that can serve as the nucleation sites for the formation of bubbles and voids, and result in swelling. Austenitic steels are known to be prone to swelling under irradiation in the presence of He while ferritic/martensitic steels are very resistant to void swelling. However, these materials suffer from embrittlement and the role that He plays on this degradation mechanism is not yet clear.

In this work we will present our progress in extending a kinetic Monte Carlo approach to include the effect of grain boundaries. An object kinetic Monte Carlo (OKMC) has been used by the authors to study He desorption during isothermal annealing from Fe samples that had been implanted with He at MeV energies. The information about defect energetics were obtained from density functional theory (DFT). In this case we focus on the effect of grain boundaries on nucleation of voids and bubbles. Values for the diffusivity of defects such as vacancies and He along the grain boundaries have also been obtained by DFT and are used as input for the OKMC model. The concentration and size of voids nucleated at grain boundaries is compared to those created in the bulk for different temperatures and He to vacancy ratios.
STRUCTURE AND STABILITY OF \(\Sigma5\) (210) AND \(\Sigma3\) (111)
GRAIN BOUNDARIES IN IRON

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High-chromium ferritic/martensitic steels attract wide attention because of their prospective applications for new generations of fusion and fission nuclear reactors. The Fe-Cr alloys serve as a model system to understand microscopic mechanism behind various processes occurring in real materials. One of such processes is the segregation/depletion of Cr at grain boundaries (GBs).

In this contribution we first investigate possible structural modifications of two GBs in Fe. In particular, these are tilt \(\Sigma5\) (210)[001] and \(\Sigma3\) (111)[-110] GBs. Using molecular dynamics (MD) quenching at zero temperature we found, respectively, totally five and three different configurations of these GBs and calculated their energies. For these purposes, the state-of-the-art interatomic potentials were utilized. Configurations obtained in this way were then relaxed by means of Vienna ab initio simulation package (VASP) and compared to the original MD configurations to confirm their stability. In addition, we also investigate the interaction of individual Cr atoms and vacancies with the lowest energy configurations of the two GBs studied in order to have a first idea which sites at the GBs attract or repulse Cr atoms and vacancies.

The most stable configuration of the \(\Sigma5\) (210) GB is employed in a companion presentation at this conference to examine the Cr segregation at this GB using a Metropolis Monte Carlo technique that takes also into account the presence of vacancies during Cr segregation.
STUDY OF IRRADIATION INDUCED BCC Nb PRECIPITATES IN THE Zr-Nb ALLOY BY AB INITIO CALCULATIONS AND MOLECULAR DYNAMICS SIMULATIONS

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The Zr-Nb alloy has been used in reactors as cladding materials and the formation of bcc Nb precipitate under irradiation plays an important role in improving the corrosion resistance of the alloy. To understand the underlying mechanism for Nb precipitate formation, ab initio calculations and molecular dynamics simulations are employed to study point defect properties and phase transition under irradiation in the Zr-Nb alloy. The ab initio calculations indicate that the formation energies of vacancy and substitutional Nb atom in alpha (hcp) Zr are much higher than that in beta (bcc) Zr, while the binding energies of the nearest neighbor vacancy-substitutional Nb pair and the nearest neighbor substitutional Nb-Nb pair in alpha Zr are smaller than in beta Zr. Moreover, the modified analytic many-body Zr-Nb potentials were presented and the potential parameters were fitted with the point defect properties derived from ab initio calculations. Applying the derived potentials, molecular dynamics simulations reveal that the alpha Zr solid solution with 15 at.% Nb transforms spontaneously into beta Zr solid solution under irradiation. These results suggest that the Nb atoms are more likely to agglomerate and form precipitates in the beta Zr than in the alpha Zr. Thus, the $\alpha$-Zr $\rightarrow$ $\beta$-Zr $\rightarrow$ $\beta$-Nb transition mechanism through in situ $\alpha$ to $\beta$ transformation of Zr and the vacancy-assisted Nb diffusion for Nb conglomeration in beta Zr under irradiation is proposed, and it explains the existence of beta Nb and Zr precipitate mixtures observed in the experiments for the Zr-Nb alloy.
EFFECTS OF CHARGES AND CHARGE TRANSFER ON DEFECTS AND DEFECT GENERATION IN CERAMICS

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Large-scale ab initio simulation methods (up to a few thousand atoms) have been developed for the study of ion-solid interactions in materials, and these methods have been employed to investigate defect properties in SiC and GaN. Atomic structures, formation energies and binding energies of small defect clusters (both vacancy and interstitial clusters) have been investigated, and their relative stabilities are determined. These results provide insights into the configurations and binding properties of these native defects. Significant charge transfer is observed to occur between carbon vacancy clusters and surrounding atoms, which results in the formation of charged defect clusters, whereas silicon vacancy clusters are uncharged clusters.

In addition, ab initio molecular dynamics methods have been used to calculate threshold displacement energies and to simulate the primary damage states for PKA (primary knock-on atom) energies up to 1 keV in SiC and GaN. These simulation results provide important insights into electronic effects on ion-solid interaction processes, and reveal that significant charge-transfer occurs between recoiling atoms. The charge variation of the PKA can decrease the energy barrier for stable defect formation, and the corresponding dynamic evolution of a stable defect is a charge-assisted process, which is expected to have significant effects on defect creation in covalent and ionic materials. Thousand-atom ab initio simulation provides a feasible path to study low-energy ion-solid interaction, charge transfer and charge-redistribution, with first-principle accuracy, in covalent materials. In addition, the migration behavior and mechanisms of point defects, with and without charge, and some small defect clusters are investigated using the nudged-elastic band method in SiC and GaN, where the atomic forces are evaluated by ab initio methods. The activation energies for these defects are determined and compared with available experimental data.
CALCULATION OF PROPER VACANCY MIGRATION ENERGY BARRIERS WITH ARTIFICIAL NEURAL NETWORKS FOR THE MODELLING OF VACANCY CLUSTERS’ MIGRATION.

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Neutron irradiation enhances mass transport in compounds via creation of point defects, thereby accelerating possible phase changes, which in turn result in material property changes. The development of predictive tools capable to model the kinetics of such processes is thus of great importance for the nuclear sector. This is a delicate issue, since it requires the accurate estimation of the mobility of defects redistributing atoms in a chemically complex system undergoing phase transformation.

The method we propose \cite{1} uses a classical atomistic kinetic Monte Carlo (AKMC) paradigm. The migration energy barrier of diffusing point defects (i.e. vacancies or self-interstitials) is calculated with only a few approximations using the nudged elastic band method, as a function of the distribution of surrounding chemical species and other nearby defects. The only required physical input is a reliable inter-atomic potential for the alloy of concern. As the use of on-the-fly calculated barriers would be unfeasible in practice, an artificial neural network (ANN) is used instead, as a mathematical regression tool, trained on a set of calculated examples. The ANN input are on-site variables describing the migrating defect’s neighbourhood.

This ANN-based approach has been successfully applied to the case of a single vacancy migrating in an alloy, i.e. with a changing chemical environment, for AKMC simulations of thermal annealing \cite{1}. The generalisation of this method for the simulation of neutron irradiation damage, requires that the existence and formation of vacancy and self-interstitial atom clusters is accounted for. In this work, we take a few steps in this direction, by considering the problem of the formation of clusters of vacancies. We find that, in order to model with the proper energy barriers all diffusion events, it is necessary to include in the model the capability of dealing with spontaneous migration events that in some cases may involve more than one single migrating atom at a time and may include diffusion jumps to distances larger than first nearest neighbours.

MOLECULAR DYNAMICS SIMULATION OF THRESHOLD DISPLACEMENT ENERGIES IN LITHIUM ALUMINATE

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During fusion reactor operation, material properties of solid breeders such as Li\textsubscript{2}TiO\textsubscript{3}, Li\textsubscript{4}SiO\textsubscript{4} and LiAlO\textsubscript{2}, are changed because of irradiation defects formed by high-energy particle irradiation. For example, decrease of the elastic property \cite{1}, which may be related to fragmentation behavior of the material, was observed by neutron irradiation. Therefore, understanding of irradiation damage processes is important so as to assure the material performance and then to deal with adverse effects appropriately. However, detailed damage processes in the materials are not necessarily revealed. For example, as far as we know, threshold displacement energies ($E_d$) of the solid breeding materials, one of the key parameters for evaluation of irradiation damage, have not been reported. Indeed, threshold displacement energies in ternary materials are not well understood.

In the present study, by using molecular dynamics technique, we aimed to evaluate $E_d$ in LiAlO\textsubscript{2}, which is a candidate solid breeding material having a relatively simple crystalline structure. A set of two-body interatomic potentials, which were constructed by fitting a model function to total energies obtained by ab initio calculation \cite{2}, were utilized.

$E_d$ was defined as the minimum energy of a primary knock-on atom (PKA) that produces a stable Frenkel defect on its own sublattice. For example, Fig. 1(a) shows “not displaced” case and (b) “displaced”. In these cases, $E_d$ was evaluated to be 46 eV.

The dependency of $E_d$ on PKA displacement direction and the average $E_d$ value over various displacement directions were respectively investigated in Li, Al and O. Correlation between the threshold displacement energies and the number of defects created with an high displacement energy (1–5 keV) were discussed.

\begin{center}
\begin{tabular}{cc}
(a) & (b) \\
\end{tabular}
\end{center}

\begin{center}
PKA trajectory \hspace{1cm} O vacancy
\end{center}

\textit{Figs. 1. Displacement of O for <100> direction with the energy of (a) 45 eV and (b) 46 eV. The final PKA position in (b) was about 0.3 nm apart from the vacancy.}

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LONG TIMESCALE MODELLING OF THE GROWTH OF RUTILE

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We will present work on modelling the surface growth of the (110) rutile TiO₂ surface. The work has used a combination of ab-initio density functional theory (DFT) and a variable charge empirical potential model to elucidate the available surface and near-surface sites and transition barriers for Ti, O, O₂, TiO and TiO₂ ad-species on the rutile (110) surface. This has led to a modified form of the potential that is capable of capturing the most important diffusion processes.

Most of the surface diffusion barriers are large in magnitude, greater than 2 eV. Thus implying that the diffusion of these ad-species would not take place on the timescale of the growth of the surface. The exception to this is the diffusion of the O atom along the surface in the [001] direction where a barrier of less than 1 eV was found. A mechanism involving interstitial Ti atoms and this O diffusion will be used to explain surface growth.

The empirical potential derived in this work has then been employed for both high temperature molecular dynamics (MD) and on-the-fly kinetic Monte Carlo (OTF-KMC). The high temperature MD has allowed us to explore a number of deposition parameters to gain insight into the experiments. We will use this to demonstrate the effects of quantities such as the deposition energy and the deposited species. The OTF-KMC, which used a combination of techniques such as the nudged elastic band and dimer methods, has been used to model the growth of the surface at realistic deposition rates. This will be used to highlight the processes that are observed during growth.
LONG TIME RADIATION-INDUCED DEFECT DIFFUSION IN IONIC SYSTEMS

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It is a fairly routine process nowadays to perform molecular dynamics (MD) simulations of collision cascades but the time scale that is accessible by MD is limited by the available computing power. The ballistic part of the collision cascade is usually over in tens of picoseconds whereas diffusion of the defects can take place over seconds or even years. Various long time scale techniques have been proposed to investigate the evolution of these defects such as temperature accelerated dynamics (TAD) and kinetic Monte Carlo techniques. For example TAD has been used successfully to investigate point defect and defect cluster mobility in MgO\(^1\).

The Monte Carlo methods require the calculation of the energy barriers for diffusion and the exponential prefactor. The exponential prefactor can be determined by the Vineyard\(^2\) method which involves the calculation of the eigenvalues at the saddle point on the potential energy surface between transitions. However in some systems such as for oxygen vacancy diffusion in \(\text{Er}_2\text{O}_3\) the saddle point calculated by the nudged elastic band or string method is a rank 2 saddle with two negative eigenvalues. This talk will illustrate how this problem can be overcome and will compare results for diffusion coefficients calculated for defects in \(\text{Er}_2\text{O}_3\) and in MgO using both TAD and Monte Carlo methods.


MULTIPHYSICS PROGRAM FOR ION-INDUCED COLLISION CASCADES AND THERMALLY ACTIVATED PHASE SEPARATION: INTERMETALLIC NANOLAYERS BY INTERFACE MIXING

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Recent developments in computational materials modelling methods have to provide a qualitatively new level of predictive power and insight into materials design. In nature, different physical processes govern simultaneously the evolution of systems. Due to the complexity of the individual processes, so far their simulations are performed separately. One key to computational progress is the multiphysical treatment in a single computer program package.

Here, we consider the evolution of interfaces under energetic ion irradiation. There, the physical process of collisional mixing is in competition with thermally activated diffusion and phase separation. We developed a novel program which treats both physical processes simultaneously. The 3D atom relocations were calculated in the Binary Collision Approximation (BCA), whereas the thermally activated relaxation of energetic, atomic configurations as well as diffusive processes, were simulated by a very efficient bit-coded kinetic 3D Monte Carlo code. Contrary to molecular dynamics simulations, our approach allows studies on experimental spatiotemporal scales.

As applications we present two extremes of interface mixing: (i) Irradiation of interfaces made by immiscible elements, here Al and Pb, with He ions causes ballistic interface mixing accompanied by phase separation. Al and Pb clusters, which form in the interface region, show self-ordering. (ii) Irradiation of interfaces made by metals which form intermetallics, here Pt and Co, with He ions causes the formation of nanometric intermetallic layers with the sequence Pt/Pt₃Co/PtCo/PtCo₃/Co across the former interface. In the element mapping perpendicular to the interface (e.g. by RBS measurements), this results in step-wise changes of Pt/Co concentrations. Novel magnetic properties of such sandwiched phases are expected. In particular, a very interesting magnetic behaviour of irradiated Pt/Co/Pt multilayers has been observed. It can be shown that the transition between out of plane and in-plane magnetic anisotropy can be triggered by ion beam irradiation, whereas computer experiment can be useful for understanding the physical mechanism.
A RECURSIVE MODEL OF DISPLACEMENT CASCADES FOR PREDICTING THE LONG Term MICROSTRUCTURAL EVOLUTION OF IRON IN RADIATION ENVIRONMENT

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ABSTRACT

Using Object Kinetic Monte Carlo (OKMC) simulations with the LAKIMOCA code, it was shown in previous work that point defect cluster size distributions at the end of 0.1 dpa irradiation of iron are independent of the PKA energy [1]. This strongly restricts the number of parameters characterizing displacement cascades and relevant to point defect cluster growth in the long term.

We performed OKMC simulations using the results of Molecular Dynamics displacement cascades as input to describe the primary damage. The cascade energy range was 10 to 200 keV, and the OKMC simulations were used to obtain point defect cluster size distributions after 0.1 dpa irradiation. We succeeded in reproducing these distributions, using randomized cascade point defect positions in cubic Confinement Volumes (CVs) with appropriate sizes instead of displacement cascades. On the basis of the results, we show that each CV may be replaced by a set of CVs each of which corresponds to lower energy cascades. Hence, cascades generated at a given PKA energy are equivalent to a set of lower energy cascades, which are in turn equivalent to a set of still lower energy cascades, and so on. This recursive picture of cascades, generalizing the concept of subcascade, is found to apply in the whole 10-200 keV energy range investigated.

THEORETICAL CALCULATIONS FOR MAGNETIC PROPERTY OF FeRh INTER-METALLIC COMPOUND IRRADIATED WITH ENERGETIC IONS

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FeRh ordered inter-metallic compound with B2 structure has been known to show magnetic phase transition from anti-ferromagnetic (AF) to ferromagnetic (F) at about 350 K.[1-3] For this compound, effects of energetic heavy ion irradiation on magnetic properties have been observed.[4] The irradiated area of FeRh changes to have ferro-magnetic moments, which means that stable AF state are broken and F state becomes stable by the irradiation. Aiming to clarify a relation between the magnetic property and a defect structure in FeRh, energy band calculations are performed based on the density functional theorem. Under an assumption that the majority of defects have a structural type of site-exchange between Fe and Rh atoms pair (inset of Fig.1), total (internal) energies for various magnetic structures are evaluated within a super-cell model of 2x2x2 cubic cells. Due to the site-exchange, internal energy increases 0.24 eV in AF structure and 0.11 eV in F structure in the cell, then the F state becomes to have lower energy than AF state. Because these values depend on the cell size, it needs to estimate intrinsic values per defect of the exchange pair. The estimated values of increase are, +1.93 eV/pair in the AF phase and +0.86 eV/pair in the F phase. From these values and an estimation of energy difference between F and AF phase[5], 0.4% of defect density gives F ground state (at zero temperature). The present calculation well reproduces the experimental result for the ion-irradiated FeRh at least qualitatively.

EFFECT OF Cr ON THE BEHAVIOR OF He IN FeCr ALLOYS FROM FIRST PRINCIPLES

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Iron based alloys play central roles in nuclear technology, in particular ferritic steels containing Cr are nowadays the strongest candidates as structural materials for future fission and fusion reactors. Although their mechanical properties have been extensively investigated, relatively little is known about the atomistic origin of their macroscopic behavior, e.g. the interplay between magnetic properties and behavior of defects in FeCr alloys. First principles calculations within the Density Functional Theory (DFT) provide such information, which is not directly accessible through experiments.

First, to check the validity of the main approximations of DFT to predict magnetic properties, we have investigated the effects of exchange-correlation functionals, pseudopotentials (norm-conserving, ultrasoft, PAW) and basis sets (plane-wave vs. localized functions) on relative stabilities of various collinear and non-collinear structural-magnetic phases of Fe and Cr. Indeed, we note that the description of Cr varies sensitively with the pseudopotentials, e.g. norm-conserving pseudopotentials tend to overestimate local magnetism in bulk Cr, which induces overestimation of the solution limit of Cr in dilute FeCr alloys.

We have then focused on the properties of He, created under high energy neutron irradiation. We aim to study the effect of Cr on the behavior of He in a model FeCr system. We have compared the formation energies of a vacancy, and a He atom at various sites in pure bcc Fe and bcc Cr, showing as results a strong dependency on the matrix material. We have studied the interaction of either vacancy or He with Cr in a Fe matrix, remarking that there is a significant repulsive interaction between Cr and He at neighboring tetrahedral site, being -0.15 eV the obtained interaction energy. Also, an octahedral He close to Cr becomes unstable falling to a nearby tetrahedral site. On the other hand there is almost no interaction between the Cr atom and either a substitutional He or a vacancy, which show similar effect on the local magnetism of neighboring atoms. We note however a slight electronic interaction between an interstitial He and either Cr or Fe, being most important with Cr, and responsible of their repulsion. Regarding the formation of small He\textsubscript{n}V\textsubscript{m} clusters close to a Cr atom, we conclude that the effect of Cr is small but for the cases where m=0. The nucleation of a five-interstitial-He cluster around a Cr atom induces spontaneous kick-out of the Cr forming a Fe-Cr mixed dumbbell, which tends to remain, bound to the resulting He\textsubscript{5}V complex.

We have evaluated as well the migration path of interstitial He and substitutional He close to a Cr atom, where the energy barriers for a tetrahedral He to jump towards a neighboring position of Cr are found to be twice larger than its migration barrier far from a Cr atom (0.12 vs 0.06 eV). Concerning the diffusion of a substitutional He via the dissociative mechanism, we find a slightly higher dissociation barrier for 1nn sites of a Cr atom. For the vacancy mechanism, by which the He atom follows the movement of a di-vacancy, we find similar diffusion properties in dilute FeCr systems and in pure Fe except a slightly lower barrier close to Cr that may induce some trapping effects.
DEFECT KINETICS IN CARBON-DOPED α-IRON: A MULTISCALE MODELING

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It is widely acknowledged that most properties of steels are primarily controlled by the presence of carbon and its interaction with point and extended defects. Resistivity recovery experiments are very useful to investigate these mechanisms occurring at the atomic scale. Indeed, after an irradiation at low temperature, a sequence of isochronal annealing sweeps in ascending order the temperature ranges where the various migration energies and binding energies between defects come into play [1]. However, the interpretation of such experiments is not always straightforward: after a strong debate on its nature, stage III in iron was eventually ascribed to vacancy migration. This has been recently confirmed in pure iron by event-based kinetic Monte Carlo (EKMC) simulations parameterized by ab initio calculations [2].

In the present study we focus on the role of carbon on the resistivity recovery measurements. We follow the same procedure as in the case of pure iron, using ab initio calculations to determine the binding energies of clusters which are then fed into the EKMC code [2]. As the number of carbon atoms remains constant over the whole range of temperature, many events have to be computed in EKMC simulations, which considerably slows down the computations. We have thus used a cluster dynamics (CD) approach at high temperature, using as input the results given by EKMC simulations. This multiscale scheme permits us to simulate the resistivity experiments within reasonable computation times.

Our ab initio calculations reveal that the SIA-C complex is energetically stable, as well as small interstitial-carbon clusters. In addition, not only the vacancy but also small vacancy clusters are strongly trapped by carbon atoms. Using these parameters, mixed EKMC-CD computations show an overall good agreement with experiments at low and high temperature, where the interaction of carbon with interstitials and vacancies dominates respectively. The trapping of SIA and small interstitial clusters on carbon leads to the disappearance of the stage related to the migration of such clusters. A strong effect of carbon is also confirmed on the vacancy migration recovery stage, which is shifted in temperature as the carbon concentration increases.

THE INFLUENCE OF STRESS ON PRIMARY DEFECT DAMAGE BY DISPLACEMENT CASCADES IN BCC IRON

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Materials for next generation nuclear reactor cores must be able to withstand more severe radiation dosages, temperatures, pressures, and chemically reactive environments as compared to current nuclear reactor cores. Advanced high-strength steels are being considered for various reactor components due to their relative neutron transparency and thermo-mechanical stability. Although there have been numerous computational studies of primary defect generation in bcc iron, only a few have investigated the influence of stress \cite{1}. The current study reports on the influence of applied stress on the statistics of primary displacement cascade defect generation in bcc-Fe using molecular dynamics simulations. Various stress levels (-1000 to 1000 MPa) are investigated for a range of primary recoil energies (1-20 keV), temperatures (0 - 600K) and stress states (uniaxial and hydrostatic). The influence of applied stress on the statistics of defect generation is found to depend on the level, state and sign of the applied stress. In general, compressive stresses have the largest influence on the total number of defects generated, whereas tensile stresses having a less pronounced influence. The effect is not linear with stress or primary recoil energy. The largest influence is observed at low primary recoil energies and intermediate applied stress. However, we find that applied stress changes the structure of the defect clusters under certain conditions. In particular, the crystallographic orientation of the dumbbell defects is polarized in a manner commensurate with the nature of the applied stress state (Fig. 1). The results are rationalized in terms of the influence of stress on defect formation energy and mobility. We also consider the influence of the non-uniform atomic stress distribution, due to the presence of the displacement cascade, on the resulting spatial distribution of the defects.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{Fig1.png}
\caption{Pole figure showing crystallographic dumbbell defect directions for a displacement cascade with a 5keV PKA energy in bcc-iron with an applied uniaxial stress of a) 0 MPa and b) 1000 MPa.}
\end{figure}

NUCLEATION OF Cu-VACANCY AND Ni-VACANCY CLUSTERS IN BCC-Fe

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Experimental investigations revealed that both the impurity Cu and the alloying element Ni may contribute to hardening and embrittlement of reactor pressure vessel (RPV) steels during the irradiation by fast neutrons. The irradiation-induced supersaturation of vacancies and self-interstitials amplifies the diffusion of the foreign atoms in bcc-Fe and causes the formation of nanosized Cu- or Ni-rich clusters which act as obstacles to dislocation motion within the grains of the polycrystalline matrix. The concentration of Cu in RPV steels is typically higher than its solid solubility and, therefore, irradiation-enhanced formation of Cu-rich precipitates is observed. Measurements showed that these clusters may not only consist of pure Cu but also include vacancies \cite{1}. On the other hand, the Ni concentration is typically below its solid solubility. That means, any formation of Ni-rich clusters, as found in \cite{2} for neutron-irradiated binary Fe-Ni alloys, is essentially irradiation-induced. Obviously, these clusters must contain additional species in order to be stable. Small-angle neutron scattering analysis \cite{2} revealed that vacancies could be the other constituent.

In the present work atomistic computer simulations using the ternary Fe-Cu-Ni interatomic potential by Bonny et al. \cite{3} are employed to investigate the thermodynamics of Cu-vacancy and Ni-vacancy precipitates in bcc-Fe. The nucleation free energy of the clusters is determined by the energy and the entropy change due to precipitation using isolated (diluted) Cu and Ni atoms as well as vacancies as the reference. In agreement with indications from measurements the nanoclusters are assumed to have the bcc structure of the iron matrix. The binding energy of the most stable cluster configurations is calculated by simulated annealing within the framework of on-lattice Metropolis Monte Carlo simulations and by subsequent relaxation using off-lattice molecular dynamics calculations.

\cite{3} G. Bonny, R. C. Pasianot, N. Castin, L. Malerba, Phil. Mag. \textbf{89} (2009) 3531.
Abstracts for poster presentations
PARAMETER OPTIMIZATION IN MD SIMULATIONS BY USING A GENETIC ALGORITHM

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Numerical simulation techniques are widely used to model physical properties or processes of various systems. For Molecular Dynamics (MD) simulations in particular, inter-atomic forces, and thus the predicted properties, depend on the quality of the force field. Therefore, the optimization of the force field parameters is essential.

In this work, we will introduce a genetic algorithm for the reactive force field developed by John Kieffer[1-5]. This potential includes directional covalent bonds, Coulomb and dipolar interaction terms, dispersion terms, etc. Important features of this force field for simulating systems that undergo significant structural reorganization are (i) the ability to account for the redistribution of electron density upon ionization, formation, or breaking of bonds, through a charge transfer term, and (ii) the fact that the angular constraints dynamically adjust when a change in the coordination number of an atom occurs.

We will present the implementation of the algorithm into the existing code as well as algorithm efficiency and preliminary results obtained for various systems. The parameters obtained by this method will be compared to existing parameter sets obtained by a trial-and-error process.

MOLECULAR DYNAMICS SIMULATION OF SURFACE DEFORMATION VIA GA\(^+\) ION COLLISION PROCESS

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The present study considers nano-order deformation of a surface when the fluence of the irradiation parameter for the calculations is set to be a realistic value for an FIB. Estimations of the deformation height from the simulation results will be important information for the crafting of nano masks by ion beam processing. Large-scale MD simulations were performed for acceleration voltages of 40 keV for Ga ions. In this work, the large-molecular dynamics simulations were performed by same program code [1] for GCIB processing with potential functions of Si. The deformation on the surface caused was analyzed after the ions collided on the Si surface. Moreover, the height of deformation was compared with the experimental value under the same irradiation conditions. The target domain is 10.7 nm × 10.7 nm × 25.9 nm, consisting of 153600 Si atoms. The initially surface was (001) crystalline at 300 K. The irradiation area is defined as 2.0 nm × 2.0 nm. At the beginning of each Ga ion impact, the Ga ion was introduced at a random location above the irradiation area on the Si surface. The Ga ion directly impacts to the Si surface without incident angle to the normal direction. The MD simulation under the regular interval impact condition was performed for the acceleration voltage of 50 keV for Ga ion. The interval time between ion impacts is defined as 199 fs that is sufficient to simulate the cooling process of the target. The surface deformation is investigated by visualizing for fluence amount of 1.0 \(\times\) 10\(^{15}\) ion/cm\(^2\), shown in Fig. 1. At Fig. 1, after a hillock structure is formed, in the upper region at the surface a few sputtered atoms were observed. A hillock structure was formed by the Ga ion impact on the Si surface. The height of the structure was found to be proportional to the fluence of Ga ions. The amorphous structural region was expanded by the progress of the interface region between the amorphous structure and the crystalline structure with increasing the fluence in the depth direction.

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Reference
CLUSTER FORMATION AT SELF-SPUTTERING OF Cu(001) SURFACE

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Nowadays the properties of matter in gas phase are well-known than the properties of matter in condensed (liquid and solid) phases. The study of clusters attempts to bridge this gap of knowledge by clustering atoms together and studying their characteristics. In present work the mechanisms of cluster formation are studied at the sputtering of Cu(001) surface by low energy grazing Cu\textsuperscript{+} ion bombardment. For this purpose a classical molecular dynamics method has been implemented using a modified Verlet algorithm to integrate Newton's equations of motions. A grazing angle of the incident particles measured from the crystal surface is varied from 5\textdegree{} to 30\textdegree{}. The number of incident particles is 100.

At grazing ion bombardment of the surface only superficial layers of the crystal have significant changes, it has caused the need for research at small angles of projectiles. Sputtering yields of the crystal surface were calculated versus the parameters of the incident ions and the results were compared with analytical calculations carried out on the basis of the cascade-hydrodynamic mechanism of sputtering. In particular it was found that the sputtering yield maxima are observed at angles to the direction along the possible channeling of the incident particles.

The energy distribution of sputtered particles was analyzed which is basic data for the study of clustering and formation of nanostructures. By analyzing the energy distributions of sputtered particles, depending on the angles of incidence of ion beam, we revealed the mechanism of cluster formation at grazing incidence and the conditions of effective cluster sputtering of the metal atoms. In addition, based on the work [1] which gives possibility of cluster formation as a result of the cascade-hydrodynamical mechanism, the probability of clusters formation with the number \( k \) of atoms in it \((k > 5)\) depending on the parameters of the incident ion were found numerically. The part of the sputtering yield due to all the clusters in which the number of atoms greater than 5 also was determined. The results are analyzed by comparison with the results obtained by computer modeling.

SYNERGY IN SPUTTERING OF COPPER NANOCLUSTERS ON GRAPHITE SUBSTRATE AT LOW ENERGY Cu₂ BOMBARDMENT

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During last fifteen years there were great number publications about synergy effect in sputtering. The effect appears as an advanced intensification of sputtering process at multiatomic particle impacts on solid surface in comparison with sum of independent sputtering processes induced by equal number of single impact atoms having the same velocity as the multiatomic particle. This effect becomes apparent, for example, in considerable increase of the sputtering yield at bombardment by metal nanoclusters [1] and fullerenes [2, 3] of the keV energies.

Molecular dynamics simulation of sputtering of clusters, consisted of 13-195 Cu atoms on a (0001) graphite surface, by 100, 200 and 400 eV Cu₂ dimers as well as by 50, 100 and 200 eV Cu single atoms have been performed. A tight binding many body potential [4] directly connected to the Born–Mayer potential was used for the Cu–Cu interactions. The Tersoff potential splined to the Ziegler–Biersack–Littmark (ZBL) potential was applied to the C–C interactions. The Cu-C interactions were simulated by the Lennard-Jones potential [5] attached to the ZBL potential.

Comparative analysis of polar angular distributions of backscattered Cu atoms, their energies as well as the energy distributions of sputtered cluster atoms at Cu₂ and Cu bombarding impacts are performed for different conditions. The reason of synergy effect in the sputtering yield and the respective sputtering energy spectra of cluster atoms are overlapping of collision atomic sequences created by each of impact dimer atoms in the surface clusters under bombardment by Cu₂ dimers as compared to two alone Cu monomers. This explanation qualitatively agrees with mechanism discussed in [6]. The curve form of low energy part of sputtering energy spectra which includes spectral maximum is basically defined by the cluster size whereas functional dependence of high energy spectra part strongly depends on energy of bombardment. This regularity is independent of type of impact particles.

MOLECULAR DYNAMICS SIMULATIONS OF LOW ENERGY ARGON ION SPUTTERING OF COPPER CLUSTERS ON POLYETHYLENE SURFACES

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Ion sputtering of 13, 27 and 39-atom copper clusters deposited on polyethylene substrates with chain folds on the surface [1] was investigated. Simulations of single normal impact events with 100-eV, 200-eV and 400-eV Ar ions were performed for each type of cluster. To get an efficient coverage of the target area, the impact points of ion were selected from a two-dimensional pseudo-random sequence.

The following interatomic potentials were used: long-range many-body AIREBO potential [2] for simulation of covalent bonding and intermolecular interactions in hydrocarbons, many-body potential [3] for simulation of copper-copper interactions, Lennard-Jones potential for copper-carbon and copper-hydrogen interactions and Ziegler-Biersack-Littmark potential for describing interaction of bombarding ions with cluster and substrate atoms. Implementations of the above mentioned interatomic potentials from the Molecular Dynamics Toolkit software package [4] were used.

Upon an increase in the bombarding ion energy sputtering yield of cluster fragments grows more rapidly for large clusters. Extrapolation of the obtained data to the region of lower bombarding ion energies indicates there is a threshold value of the energy required for the sputtering of substrate atoms. The bombardment of bigger clusters is characterized by greater values of the backscattering coefficient.

Atomic hydrogen prevails by number of particles in the yield of compounds composed of atoms initially resided in the substrate. The yield also contains a considerable amount of acetylene, methylene, methine and other hydrocarbon radicals.

Single atoms of copper predominate among the sputtered fragments by number of particles in those cases where the bombarding ion interacts with the cluster atoms prior to possible interaction with the substrate. Where there was no substantial interaction between the cluster and the bombarding ion prior to its collision with the substrate, mostly intact cluster sputtering from the substrate surface was observed.

Most of the sputtering occurred during the first 3 ps after the impact. After 3 ps we observed the slow desorption of clusters (often having already lost a small number of their atoms in the first 3 ps), along with the sputtering of large fragments of polyethylene chains and other heavy hydrocarbon compounds.

EFFECT OF IMPACT ANGLE AND PROJECTILE SIZE ON SPUTTERING EFFICIENCY OF SOLID BENZENE INVESTIGATED BY MD SIMULATIONS

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Molecular dynamics computer simulation is used to investigate the effect of projectile size and impact angle on the efficiency of surface erosion. 14.75 keV argon clusters Ar\textsubscript{n} (n=366, 872, 2953, 9000) are directed at the surface of a coarse-grained solid benzene crystal at angles between 0 and 70 degrees. It has been observed that the shape of the angular dependency of surface erosion is strongly affected by the cluster size. For small and medium size clusters Ar\textsubscript{366} and Ar\textsubscript{872} the sputtering yield only slightly increases with the impact angle, has a broad maximum around 40 degrees, and decreases at larger angles. For large clusters, the yield strongly increases with the impact angle, has a maximum around 45 degrees, and steeply decreases at larger angles. It has been found that for all clusters the primary energy is deposited at the optimum depth. As a result, the sputtering efficiency only weakly benefits from shifting the energy profile closer to the surface observed at larger impact angles. This process is mainly responsible for a strong signal increase with the impact angle observed during atomic, and small cluster bombardment. At larger impact angle sputtering efficiency decreases due to increased effect of primary energy being backreflected into the vacuum. A strong increase of the sputtering yield with the impact angle observed for Ar\textsubscript{2953} and Ar\textsubscript{9000} clusters is attributed to the washing off mechanism stimulated in solid benzene by a flux of redirected Ar atoms. We believe that this mechanism is important for large cluster projectiles irradiating weakly bound solids.
COMPUTER MODELLING OF CONTINUOUS BOMBARDMENT OF AG(111) BY KEV C_{60} CLUSTERS

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We shall present a theoretical insight into processes taking place during continuous irradiation of Ag(111) surface by keV C\textsubscript{60} projectiles. Molecular dynamics simulations are employed to probe energy deposition patterns, accumulation of ion induced damage and evolution of the surface morphology within a projectile fluence of $5 \times 10^{14}$ cm\textsuperscript{-2}. The initial conditions include a range of incident energies and angles used in secondary ion and neutral mass spectrometry (SIMS/SNMS) experiments. A special emphasis is placed on probing the processes that determine the depth resolution in depth profiling SIMS/SNMS experiments. It is shown that bombardment events on the damaged surface exhibit a diversity of dynamics not observed on flat surfaces.
STOPPING OF CLUSTERS IN SOLIDS

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Molecular-dynamics simulations of cluster impact on solid surfaces have been performed to provide information on the stopping forces and deformation of these clusters. We investigate the dependence of these quantities on the impact energy and the cluster size. We consider self-bombardment of an Ar and a Cu system. For a frozen amorphous Ar target, we investigate cluster sizes of 13, 100 and 1000 atoms and total impact energies of 0.1 – 4 keV. For a crystalline Cu target with (100) surface the cluster sizes are 43, 100, 1000 and 10000 atoms with total impact energies of 1 – 10000 keV. Our simulations show that the stopping force $dE/dz$ rises sublinearly with the impact energy $E$ per atom: $dE/dz \propto E^\alpha$. For both systems, the exponent $\alpha$ is in the range 0.5 – 0.8 with only slight dependence on cluster size $N$. Our data also show a distinct dependence of the stopping force on the cluster size $N$: $dE/dz \propto N^{1-\beta}$ with $\beta$ in the range 0.3 – 0.4 for both Cu and Ar with no significant dependence on $E$.

When the cluster is decelerated in the solid target it becomes deformed in vertical direction. We measure this strain as the ratio of the actual vertical extension and its original value. We define as strain rate $\mu$ the maximum of the time derivative of the strain. We find that in an restricted low-energy regime, the strain rate is proportional to the impact velocity: $\mu = \gamma v$ with $\gamma$ decreasing from 2 to 0.5 km$^{-1}$. For small clusters at high energies, the strain rate assumes smaller values than predicted by this law; this is due to the fact that for the smallest clusters at high energies cluster fragmentation and individual cluster-target atom interactions become more pronounced, an effect that also has to be paid attention to for the stopping force.

Fig. 1. Cu$_{10000}$ Cluster (green) getting stopped in a Cu crystal  Fig. 2 Stopping analysis of Ar$_{100}$ at 1 keV in Ar
TOPOGRAPHY SIMULATION OF SPUTTERING USING AN ALGORITHM WITH SECOND ORDER APPROXIMATION IN SPACE

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Focused ion beam milling is an established technique for many nanopatterning applications. Moreover, existing micro- and nanostructures are modified by conventional ion milling. For the efficient simulation of these processes continuum surface advancement algorithms are used. In two-dimensional algorithms the surface is represented by a string of points connected by straight line segments. In this work we present an algorithm that uses circular arcs between data points and, moreover, allows kinks in the surface for the simulation of shocks.

The algorithm is based on the method of characteristics [1], which yields the motion of the points and the slope of the surface. By the interpolation with circular arcs not only the final result is better represented, but also more accurate simulation is possible after insertion of new points as the surface evolves. In addition, we have derived a criterion for the generation of shocks by analyzing infinitesimally separated characteristics. It requires the curvature of the surface, which may readily be determined from the radii of the circular arcs. The motion of these shocks is treated as in Ref. [1]. As an example, in Fig. 1 the evolution of the surface under a Gaussian beam is shown. The characteristics are shown by dotted lines. After the fourth time step four shocks are generated indicated by the red circles.

The proposed algorithm uses a second order approximation in space and therefore requires fewer data points during calculation. This is particularly important when redeposition is included, as the computational effort for redeposition is quadratic with the number of points. The algorithm is, in principle, extensible to 3D, where the number of points is quadratic with the resolution.


Fig. 1: Surface evolution under a Gaussian beam. Blue lines indicate the surface, dotted lines characteristics, and red circles shocks.
ION MILLING AND ION IMPLANTATION IN MBE MCT

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At present time the most perspective material for infrared photodectors manufactured are epitaxial films Hg$_{1-x}$Cd$_x$Te (MCT) with varied gap layers near surface region and in the volume of the material. The ion implantation and ion beam milling (IBM) are widely used for the creation heterogeneous semiconductors structure, such as p-n junction. The irradiated MCT material main feature is that all properties (electrophysical, optical, etc.) are completely determined by radiation defects (RD). For acknowledging usability of the ion doping and ion milling processes reference to varied gap MCT epitaxial films it is necessary to investigate the RD formation and evolution processes at region where variation composition of the MCT material is observed.

In this work experimental results of electrical active radiation defects formations on boron implantation and ion beam milling (Ar$^+$) of the p-type MCT epilayers with various composition ($x_s$) distribution near surface area of the material is presents.

For the experiments the epitaxial films with various composition distribution near surface ($x_s$) have been grown specially. As-grown film had n-type with concentration $\sim 2 \times 10^{14}$ cm$^{-3}$ and mobility $\sim 5 \times 10^4$ cm$^2$V$^{-1}$s$^{-1}$. For p-type manufacturing the films was annealed in a neutral ambient of hydrogen or helium. After anneal the hole concentration in MBE MCT films at $T = 77$ K was $p = (3-8) \times 10^{15}$ cm$^{-3}$, hole mobility $\mu_p = (480-560)$ cm$^2$B$^{-1}$s$^{-1}$. The ion beam milling at a room temperature was carried out by ions Ar$^+$ with energy 0.5 keV, within 5–20 minutes at a current density $j = 0.1$–0.3 mA/cm$^2$. The boron implantation was carried out at a room temperature, the interval of doses and energies were $10^{11}$–$3 \times 10^{15}$ cm$^{-2}$ and 20 – 150 keV, respectively. The ion current density was $j = 0.001$ – 0.2 $\mu$A·cm$^{-2}$. The postimplantation annealing was not carried out. The measurement of the electrophysical parameters before and after irradiation was at 77 K by a Van der Paw method.

The donor type RD spatial distribution in the surface region of the material after irradiation are analyzed. The electrophysical measurements of the irradiated samples has shown, that the after irradiation the conversion type conductivity is occur because of high doped n$^+$ layer formation near the samples surface. The results comparison of boron ion implantation and IBM has shown essential difference in the donor centers spatial distribution depending on a composition of surface layer ($x_s$). The common property of both process is that as IBM (at all regimes), and the high doses boron implantation ($10^{14}$–$3 \times 10^{15}$ cm$^{-2}$) form the n$^+$/n$^-$/p structure independently of a composition $x_s$. However essential difference in depth n$^+$ and n$^-$ layers and an electron concentration is observed.
DEPTH DISTRIBUTION OF THE COBALT IN RUTILE (TiO₂) IMPLANTED TO HIGH FLUENCES

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Transparent diluted magnetic semiconductors (DMS) represent a new class of magnetic materials perspective for spintronic and magneto-optic applications [1]. Ion-beam implantation with magnetic 3\textit{d} ions is a promising technique to synthesize the desired DMS [2]. In the above context, (100)- and (001)-monocrystalline plates of semi-conducting rutile (TiO₂) were implanted with 40 keV Co\(^{+}\) ions to fluences of \((0.15–1.5)\times 10^{17} \text{ ion/cm}^2\) at room (300 K) or high temperatures (600 or 900 K). The samples reveal room temperature ferromagnetism caused by formation of two magnetic phases: Co nanoparticles and the solid solution of Co ions in the rutile structure [3]. In this report we present results on anomalous depth distributions of cobalt ions in TiO₂ substrates implanted along the structural channels at high temperatures. We succeeded in modeling of the experimental depth profiles taking into account anisotropic diffusion of the cobalt ions and their precipitation on different accumulating centers.

To find the implant distribution \(N(z,t)\) as a function of the depth \(z\) and the time \(t\), one-dimensional diffusion equation with the steady source of the implant ions had been used. The spatial distribution of the stopped ion source was simulated by the Gaussian profile centered around the projected range \(R_p\) with the straggling \(\delta R_p\). The initial condition \(N(z,0) = 0\) (the absence of implant in the substrate till the implantation process started) and the bounding requirement \(\partial N(vt,t)/\partial z = 0\) (the absence of the implanted ions backflow through the facade surface) were utilized to find the integration constants of the diffusion equation. The surface sputtering effect was taken into account by the uniform motion of the source into the substrate depth with the velocity \(v\). The presence of the precipitation centers was formalized by introducing drain terms into the diffusion equation.

The computed depth distribution profiles fit well the experimental profiles of cobalt ions in TiO₂ obtained from Rutherford backscattering measurements. The physical parameters of the model, such as diffusion constants at three temperatures of the substrate, 300K, 600K, and 900K, agree well with the data of other studies of cobalt diffusion in rutile. Based on our calculations we succeeded in explaining the unusual concentration peak deep in the sample appearing at elevated substrate temperatures. Moreover, the model allowed to separate various contributions to the samples magnetization originating from different dopant phases. This result agrees well with the two-phase model of magnetism in Co-implanted TiO₂ [3].

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THE EFFECT OF SOME EFFECTIVE QUANTITIES TO ELECTRONIC STOPPING POWER

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Abstract
The dependence of effective quantities $Z^*$, $Z^†$, $I^*$, (effective number of electrons for ionization and for quasi-molecule, effective mean excitation energy), on the incident ion energy have been studied for a pervious stopping power calculation method (Gümüş and Köksal, (GK) method), and Bohr stripping criterion and quasi-molecule criterion in this regard have been discussed in some details. The effect of effective quantities to the obtained stopping power results is investigated by calculating stopping powers. The contribution to stopping power from the modified LSS and Bethe formulas have been calculated separately and compared in graphs of stopping power.

Key words: Stopping power; effective mean excitation energy; effective number of electrons; Li ion.
APPROACHES FOR DEVELOPMENT OF FAST MONTE-CARLO CODE FOR CALCULATION OF THE ELECTRON STOPPING IN SUBSTANCE

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The first step of standard Monte-Carlo codes of electron trajectory simulations [1] in a substance with atomic density \( n \) and atomic number \( Z \) is calculation of the mean free path \( \lambda = \frac{1}{n\sigma(k)} \) for the given electron energy \( E = \frac{1}{2}mk^2 \). Here \( \sigma(k) \) is the total cross-section of electron scattering on atom. The real path length is found from the relation \( x = \lambda \ln(1/\xi) \), where \( \xi \) is the random value with the uniform distribution on the interval (0,1). In classical physics \( \sigma(k) = \infty \) [2], henceforth, \( \sigma(k) \) has the quantum-mechanical nature. The main contribution to it comes from large impact parameters, \( \rho \approx a_0Z^{1/3} \), where \( a_0 \) is the Bohr radius. So, \( \sigma(k) \) is dominated by electronic shells of atom. It results in very small \( \lambda \) values and time-consuming of Monte-Carlo code. At the same time, it is known [1] that in the practically interesting case \( Z \ll 1 \) the scattering of the electron beam is dominated by the collisions of electrons with nuclei taking place at \( \rho \approx a_0Z^{1/3} \), which, at the same time, are characterized by small scattering angles. Therefore, there is no reason to use above mentioned slow standard Monte-Carlo method. The alternative method is presented in the report that originates from plasma physics. It is based on the diffusion-like character of the electron scattering and is characterized by \( 5 \div 10 \) times larger typical values for path length \( x \) values. The resulting Monte-Carlo code is much faster than standard one and has approximately the same accuracy. Some results for the 30 KeV beam and half-space copper target are given in Figures 1 and 2. Distribution functions are presented in arbitrary units.
SIMULATION OF INCOHERENT BREMSSTRAHLUNG IN FLAT AND DEFORMED CRYSTALS

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The bremsstrahlung cross section for relativistic electrons in a crystal splits into the sum of coherent part (due to the periodicity of the spatial arrangement of atoms in the crystal) and incoherent one (due to a thermal motion of atoms in the crystal) [1]. Although the spectrum of incoherent radiation in crystal is similar to one in amorphous medium, the electrons’ flux redistribution in the crystal (channeling etc.) could lead to substantial dependence of the incoherent radiation intensity on the crystal orientation. The simulation based on the semiclassical description of the radiation process [2] had confirmed that viewpoint. The results of simulation are in a good agreement with the corresponding early [3] and recent [4] experimental data.

Here we present the improved simulation procedure taking into account the crystal deformations. The simulation was carried out under the conditions of the recent experiment performed at the Mainz Microtron MAMI [5] to explore the radiation emission from periodically bent crystal. The results of simulation demonstrate qualitative agreement with the experimental data. The decrease of the radiation intensity in comparison to the reference flat crystal permits to estimate the reduction of the dechanneling length due to the crystal bending.

![Fig.1. Results of simulation for the incoherent bremsstrahlung intensity (in ratio to Bethe-Heitler intensity in amorphous medium) from 855 MeV electrons in flat (left plot) and sinusoidally bent (right plot) silicon crystals under scanning of the goniometric angle like in the experiment [5]](image)

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COMPARISON BETWEEN MONTE CARLO AND EXPERIMENTAL ALUMINIUM AND SILICON ELECTRON ENERGY LOSS SPECTRA

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A Monte Carlo simulation is described and used to calculate the energy distribution spectra of backscattered electrons from Al and Si. Elastic scattering cross section calculations are performed by numerically solving the Dirac equation in a central field. Inelastic scattering cross sections are evaluated in terms of a Drude-Lorentz dielectric function. Extension from the optical case to non-zero momentum transfer is done according to Ritchie and Howie [1]. To evaluate surface and bulk contributions to the spectra, the Monte Carlo model treats the surface excitations according to the Werner [2] differential surface and volume excitation probability theory. The Monte Carlo calculations are compared with the experimental reflection electron energy loss (REEL) spectra acquired in our laboratory.

BACKSCATTERED ELECTRONS FROM SURFACE FILMS DEPOSITED ON BULK TARGETS: A COMPARISON BETWEEN COMPUTATIONAL AND EXPERIMENTAL RESULTS

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It is well known that over-layer films affect the electron backscattering coefficient of bulk targets, in particular for primary energies lower than 3 keV. In this primary energy range, the experimental data available in the literature for backscattering coefficient are rather scattered and some difficulties arise in their interpretation due to the lack of knowledge of the thickness, uniformity, and nature of the surface layers. In particular, a quantitative treatment of the effect of surface films deposited on bulk targets and a systematic comparison with experimental data are currently lacking. In this work, a Monte Carlo code is briefly described, validated, and utilized to calculate the backscattering coefficient from surface layers deposited on bulk targets of different nature and composition. A quantitative evaluation of the backscattering coefficient as a function of the over-layer thickness is provided, as well as a comparison of the simulated results with experimental data concerning thin films with known thicknesses and compositions.
KINETIC EXCITATION OF SOLID SURFACES: THE INFLUENCE OF PROJECTILE IMPACT ANGLE

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We present a computer simulation study on the kinetically induced electronic substrate excitations generated during self-sputtering of a metallic surface. For the example of a silver target bombarded with 5-keV Ag atoms, a standard molecular dynamics code is employed to follow the microscopic particle dynamics within the atomic collision cascade following the primary particle impact. The conversion of kinetic energy of cascade atoms into the electronic subsystem of the metal is treated in terms of the Lindhard model of electronic stopping and an electron promotion model describing the generation of hot electrons in close binary collisions, while the transport of excitation energy away from the spot of generation is treated in a diffusive manner. The calculations yield a time- and space-dependent excitation energy density profile that can then be used to describe inelastic ion-surface interaction processes such as ion induced electron or secondary ion emission.

The focus of this study is set on the influence of the impact angle (with respect to the surface normal) under which the projectile impinges onto the surface. For different polar angles of incidence, sets of 169 trajectories - each corresponding to one particular impact point of the projectile on the surface - have been followed and analyzed to discuss the resulting electron temperature profiles. It is shown that oblique incidence leads to a strongly modified excitation profile which is centered closer to the surface than under normal impact.
NUMERICAL STUDY OF FORMATION MECHANISMS OF PERIODIC SURFACE STRUCTURES INDUCED ON SILICON UNDER FEMTOSECOND LASER IRRADIATION

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Multiple irradiation of bulk silicon target by several femtosecond laser pulses (λ=800 nm) at sub-threshold ablation energies lead to the formation of several well known types of microstructures. With few laser shots, sub-wavelength periodic structures named ripples appear [1]. With more laser shots, they merge to form drop-like and viscous structures named beads. At higher number of shots, these structures lead to the formation of micrometric-sized cones. The cones randomly distributed form the so-called “black silicon” for its great absorption properties of visible light that can be used to increase the efficiency of silicon photovoltaic cells [2,3] and photodiode detectors.

In the present work, we present the results of a modeling study based on two temperature model and carrier generation equations that was performed to describe the effect of several femtosecond laser pulses acting on a surface of Si. Simulations take into account such processes as melting, phase front moving, cooling and re-solidification. In this approach we consider at first, the formation of ripple structures (Fig. 1a) by electromagnetic waves diffraction and interference [4,5,6], and nanofluidic capillary wave excitation [7]. Then, we describe the coalescence of these small structures to the larger bead-like structures (Fig. 1b), and explore a mechanism based on capillarity forces explaining the self-organized pattern (Fig. 1c) observed after spike formation (Fig. 1d).

![Figure 1](image_url)

**Figure 1 :** Modification of surface structures while increasing number of pulses with 100 fs, 800 nm laser irradiations.

MONTE CARLO CALCULATION OF ELECTRON DOSE POINT KERNELS IN WATER USING DIFFERENT TRANSPORT APPROXIMATIONS

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The spatial distribution of absorbed energy in irradiated matter can be conveniently described by dose point kernel (DPK) distributions that characterize the average energy deposition around single charged-particle tracks during their slowing down process. In the present work we use Monte Carlo simulation of electron transport in unit-density water to investigate the effect on DPKs of different transport approximations in the energy range from 100 eV to 100 keV. We consider three approximations to the (electronic) energy loss problem: (i) the single-scattering scheme whereby all inelastic collisions are individually simulated, (ii) the continuous slowing down approximation (CSDA) whereby the energy loss is determined from a suitable stopping power formula, and (iii) the mixed-transport scheme which combines single-scattering simulation for hard inelastic collisions and the continuous approximation for soft inelastic collisions. In all schemes, elastic collisions are individually simulated using the screened Rutherford formula with empirical Mott corrections. The inelastic cross sections used in the present work are obtained from a relativistic Bethe-like expression with parametric empirical oscillator strength distribution and Fano’s approximation for the transverse interaction. For the CSDA scheme we use the relativistic Bethe stopping power formula above 10 keV and examine different phenomenological expressions at lower electron energies. In the mixed-transport scheme a restricted form of Bethe’s stopping power formula is used to model the energy loss from soft inelastic collisions and Möller’s cross section is used to describe hard inelastic collisions. Our findings indicate that the DPKs are increasingly sensitive to the above approximations with decreasing electron energy, with the mixed-transport scheme being in fair agreement with the detailed simulation above about a few tens of keV.

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HYBRID CONTINUUM-ATOMISTIC SIMULATIONS FOR ULTRASHORT PULSED LASER ABLATION

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The increasing number of laser ablation applications requires research to understand the very fundamentals of laser-solid interactions. In this study, we investigate the effect of an ultrashort (~100fs) laser pulse on metal, using a hybrid continuum-atomistic model. Phase transitions are analyzed.

The model we use [1,2], is a combination of the two temperature model (TTM)[3] and a molecular dynamics (MD) approach. The trajectories of the atoms are obtained by solving Newton’s equation in a Verlet scheme. Hence, we can obtain the lattice temperature. The electronic temperature is calculated by a continuum equation and solved by a finite volume scheme. Both equations are coupled. A big advantage of the atomistic approach, compared to the only-TTM, is that phase transitions at these extreme non-equilibrium conditions can be studied.

In order to simulate the laser-solid interaction on the surface of a metal, a large grid should be used, so that the calculated properties at the bulk boundary remain in their initial bulk state. Whereas temperatures are calculated with the TTM for the entire grid, which is 500nm, the MD part is only used in the first 100nm of the simulation cell, in order to reduce computational time. This creates some inner boundary in the simulation. Recently, our research group made an improvement to the hybrid model by including a ‘moving boundary’ (MB) at 100nm [4]. The MD box expands at the inner boundary, as a result of the thermal expansion of the metal. Therefore, the boundary will move towards the bulk side. This MB replaces the addition of new cells in the surface region.

Our simulations show a direct solid-to-vapor transition. The evaporation of the solid surface material goes layer-by-layer. The very small amount of liquid material will reduce the liquid splashing and crater formation around the ablated hole. In this manner, very clean microholes can be drilled. This behavior corresponds to experimental work [5,6].

MECHANISM OF ANISOTROPIC DAMAGE CREATION AROUND THE TRACK OF A SUB-SURFACE CHANNELED ION

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Using molecular-dynamics simulation we investigate the anisotropy of the adatom distribution on the sides of channeling tracks after a sub-surface channeling event of keV Xe+ ions in a Pt(111) sub-surface channel. This behavior is found when an ion channels in [1-10] direction, along a dense atomic row. Instead of an open planar channel, the ion encounters an axial channel between two planes. Due to the relatively large size of the Xe atom and the steering of its motion by the smooth axial-channel potential, the ion is able to remove completely the surface atoms in one to two rows. The track of such an event is visible by an STM apparatus.

The profile of the sub-surface channel controls, as well, the polarization of the oscillatory ion motion. As a consequence, the adatoms are distributed asymmetrically on different sides of the trajectory. This behavior can be explained by a simple geometrical picture of the target crystal. When the channeled ion collides with the very first surface layer, it pushes the surface atoms out of their positions into adatom sites, mostly to the left of their positions. As a result, the ion leaves a distinct track on the surface: it consists of a vacancy groove decorated by adatoms which concentrate on the left side.

(a) STM topographs after exposure with 5 keV Xe+ ions incident at $\theta = 86^\circ$. (b) Top view of MD simulation, (c) simulated ion trajectory.
MOLECULAR DYNAMICS SIMULATION OF NANOSCALE TRACK FORMATION BY SWIFT HEAVY IONS IN ZIRCON

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Zircon is a candidate ceramic waste form for nuclear-waste immobilization and is used in thermo-chronology to unravel Earth's history. We have simulated the passage of swift heavy recoils through a zircon crystal and the subsequent annealing with classical molecular dynamics using the thermal-spike model. We created thermal spikes changing the initial ion velocities that corresponded to a certain energy loss per unit length (dE/dx). The dE/dx range simulated was from about 2.5 to 13 keV/nm. The thermal spike was in the form of a cylindrical track of 3.0 nm radius. Damage to the crystalline lattice recovered completely when the thermal spike energy was below 2.5 keV/nm. These simulations establish a threshold dE/dx for fission-track formation in zircon and show that the fission-track radii also depend considerably on the magnitude of electronic energy loss (dE/dx).
NANOCLUSTER MODIFICATION BY SWIFT HEAVY ION TRACKS

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Elongation or flattening of metal and semiconductor nanoclusters inside an insulating substrate has recently been demonstrated on several materials under swift heavy ion irradiation. The effect has been shown to be related to swift heavy ion track formation properties of the substrate. In recent experiments, a previously unresolved fine structure in ion tracks in amorphous silica was found comprising a low-density core and a high-density shell, and was confirmed by molecular dynamics (MD) simulations [1].

The origin of the fine structure is a picosecond time scale pressure wave out of the track center, creating a temporary low-density region around the ion path in several materials, and the observed nanocluster shape transformations may be closely linked to the process.

We present large-scale MD simulations on amorphous silica, and systems with Au and Ge nanoclusters under swift heavy ion irradiation, showing how the dynamics of track formation in the substrate and nanocluster material and dimensions affect the cluster shape transformation.

![Elongation of a 6 nm gold nanocluster after a single 22 MeV Au ion](image)

Fig. 1. Elongation of a 6 nm gold nanocluster after a single 22 MeV Au ion

SPATIO-TEMPORAL DYNAMICS OF ION TRACKS IN SILICON

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The track structure created by a swift ion passing through a semiconductor material causes different physical effects such as single-event-upsets (SEUs), radiation damage including sputtering, and local modification of the solid state phase. These effects depend on the spatial distribution and on the timing of the evolution of the electronic and atomic subsystems after the passage of the ion. In this presentation, we will consider only the characteristics of the cascading electrons created by the primary $\delta$-electrons ejected by the ion into the bulk of silicon. This stage extends in time from 0.1 fs up to 10 ps and radial distances from the track axis up to the maximal range of the $\delta$-electrons (up to 10–20 $\mu$m, depending on ion energy). Experimentally, one can investigate only the post irradiation effects and the prehistory of these events can be simulated using Monte Carlo (MC) or molecular dynamics (MD) calculations.

Our MC calculations are based on a self-consistent physical model (see [1,2] and references therein). One of the results obtained in these calculations shows that the spatial and temporal track-structure evolution are mutually dependent and cannot be considered separately. Nevertheless, this separation has been commonly used, for example, in the thermal spike model [3]. In Fig. 1, the radial distribution of the deposited energy for different times $D(r, t)$ (in eV nm$^{-3}$ s$^{-1}$) is shown for 10 MeV/amu protons. For heavier ions, the energy should be multiplied by $Z_{\text{eff}}^2$ ($Z_{\text{eff}}$ is the effective ion charge). Fig. 2 shows the radial distribution $D(r)$, after integration of $D(r, t)$ over time. It is clear that the results in Fig. 1 cannot be obtained by multiplying the curves in Fig. 2 by any temporal function. The full article will present, for ions of 1–100 MeV/amu, the spectra of hot electrons, the numbers of stopped electrons (those reaching $E < 1.5$ eV), the track radii, and other results – as well as a comparison with existing experimental data.

Fig. 1. The radial distribution of the deposited energy by 10 MeV protons for different times. Fig. 2. The total radial distribution for protons with different energies.

Irradiation with swift heavy ions in some dielectric materials has been shown to induce structural disorder, including amorphization, that presents clear differential features with regard to that caused by nuclear collisions. Recently, lattice compaction (densification) and point defect formation have been induced at the surface of a-SiO₂ by irradiation with F, Cl and Br in the electronic stopping regime. The densified layer results from the overlapping of the tracks generated by single ion impacts so that the average increase in density depends on irradiation fluence. The compactation was measured through the light propagating modes along the higher refractive index surface layer. It is often assumed that those tracks are produced via the high-temperature temperature rise around the ion trajectory (thermal spike). In this communication we have used MD simulations to describe the effect of the shock pressure wave associated to the high thermal gradient at the spike as well as the effects associated to overlapping of near-by impacts. Moreover, the same aproach has been used to investigate the structural disorder (bond rearrangement and breaking) that may be also induced during irradiation. The objective is to ascertain whether the two effects (compaction and disorder) can be understood within the same thermal spike model.
MODELING DAMAGE ACCUMULATION IN FE AND FE-CR ALLOYS IRRADIATED WITH IONS

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The evolution of the microstructure in ion-irradiated Fe and Fe-Cr alloys is studied using kinetic Monte Carlo models with input from other simulations, mainly density functional theory and empirical potential calculations. Experimentally two type of defects are observed when these materials are irradiated with ions, ½<111> and <100> loops. However their nucleation and growth is still not completely understood.

In this work we present a kinetic Monte Carlo model for damage evolution in ion-irradiated Fe. Information about defect energetics, such as migration energies or binding energies of defects to clusters come from either density functional theory when available or from empirical potential calculations. In a first approximation, we consider that <100> loops nucleate from the interaction of two 1/2<111> loops, as first proposed by Marian et. Al [1]. Using this model we study the concentration of defects as a function of dose as well as the ratio of 1/2<111> to <100> loops and the size distribution of each type of loop. To test the validity of the model, results are compared to experimental simulations. The effect of Cr is then included in an effective manner. It is known from simulations that the presence of Cr affects the mobility of 1/2<111> loops. Therefore, using the model for pure Fe we study the effect of the mobility of these clusters in the defect concentration as a function of dose as well as defect distribution.
SIMULATION OF END-BRIDGE-LIKE RADIATION DEFECTS IN CARBON MULTI-WALL NANOTUBES

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One of the main goals of using nanotubes in making new materials as reinforcement components is using their extremely high mechanical properties in combination with low density. But it should be taking into account that the sp² electron structure often results in very low binding energy between CNT’s surface and atoms of many different matrices with sliding between MWNT’s elements under stressed state. In this situation modifying a structure by introduction a number of cross-linking defects can improve situation and increase the stiffness of the MWNT’s fragments and their binding with a matrix. The paper presents results of computer simulation and theoretical study of some stable configuration of bridge-like radiation defects which can be produced under fast electron or ion irradiation in multiwall nanotube fragments which are free or introduced into a matrix. As especially interesting result we should notice formation of unusual tubular nanostructure after closing an initially open gap between MWNT’s inside and outside tubes by end-bridge-like defects. The binding energies and structure characteristics of some stable configurations of defects, were determined by using the well known semi-empirical extended Hückel techniques and the density functional theory. Results of computer modeling and calculations show, that radiation modifying of carbon nanotubular structures with forming bridge-like defects can provide essential increase of strength and stiffness of the composite material.

Figure 1. Atomic configuration of the end-bridge-like defects in a two-walled carbon nanotube
FIRST-PRINCIPLES STUDY OF POINT DEFECTS AND OXYGEN SELF-DIFFUSION IN URANIUM DIOXIDE

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Uranium dioxide UO₂ is the standard nuclear fuel used in current pressurized water reactors. The description of this oxide by first-principles calculations remains challenging because of the peculiar properties of the uranium 5f electrons which do not allow the standard LDA or GGA functionals to accurately reproduce its electronic properties.

In this study, we use the DFT+U approximation to take into account the strong correlations among 5f electrons and we first investigate the stability of the Jahn-Teller distortion in UO₂ seen experimentally at low temperature [1]. We also study the relative stability of the collinear (1k) and the noncollinear (3k) antiferromagnetic orders, taking into account the spin-orbit coupling.

Second, in order to better understand the behavior of uranium dioxide under irradiation, we investigate the stability and migration mechanisms of point defects, in particular oxygen defects, whose excess governs radiation tolerance, as well as fission product accommodation and release. Activation energies for oxygen self-diffusion have already been measured and reported in the literature [2-5], but still little is known about migration mechanisms. We therefore determine the formation energies various point defects in UO₂, and we compare the results obtained in the fluorite structure with those in the Jahn-Teller distorted structure. We finally calculate migration energies for oxygen defects using the Nudged Elastic Band method [6]. We investigate simple migration pathways, such as the interstitialcy and direct mechanisms for the single interstitial, as well as diffusion along the [100] and [110] directions for the single vacancy.

Using formation and migration energies calculated, we determine the activation energies for oxygen diffusion in UO₂ and compare our results with recent DFT [7] and DFT+U results [8], as well as with new experimental values determined by electrical conductivity measurements. In order to prevent the system from reaching metastable states created by the DFT+U approximation, all calculations are carried out using an efficient scheme based on the control of uranium 5f occupation matrices [9].

References
MODELLING He IN Pu

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The formation of He bubbles in metals subjected to radiation damage is known to have a number of significant effects, including inducing swelling and a degradation of the mechanical properties of the material. The work presented in this paper will discuss the properties of He and He bubbles in Ga doped δ-Pu and their interaction with self-irradiation.

Results will be presented on the energetics of He defects in Ga doped δ-Pu and barriers for He migration in the system. Work on the use of on-the-fly kinetic Monte Carlo (kMC) to study the diffusivity of He will also be presented. This will highlight the role of both vacancies in the system and the distribution of Ga in the system. The results of this study have significant implications for the formation of He bubbles in Ga doped Pu.

The results of a study of the energetics He bubbles as a function of both the bubble radius and the He-vacancy will then be presented. These results allow the identification of the most stable He-vacancy ratio as a function of bubble size. The results presented will also show how the energy per He atom varies as a function of bubble size, highlighting what are the most stable He bubble sizes.

Finally work on the interaction of radiation damage with He bubbles will be presented. This work will illustrate how the size of a He bubble can grow due to capturing vacancies formed as a result of a collision cascade. They also show that if a collision cascade occurs near a He bubble then the amount of residual damage in the lattice can be larger than expected due to the bubble absorbing vacancies that otherwise would have annealed with interstitials.
**AB-INITIO MODELLING OF W-Ta AND W-V ALLOYS FOR FUSION APPLICATIONS***

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Design of materials tailored for specific applications is the central objective of materials engineering. Recent progress in density functional theory modelling now makes it possible to predict properties of materials using atomic-scale simulations. These simulations provide information about the phase stability of materials as a function of chemical composition, as well as about the formation and migration energies of radiation defects, which are difficult to measure experimentally.

In this study, we investigated the phase stability of tungsten-based alloys W-Ta and W-V, and the structure and formation energies of radiation defects in these alloys. Tungsten-tantalum and tungsten-vanadium alloys are candidate materials for DEMO divertor applications because of their high melting point and expected improved ductility and fracture toughness in comparison with pure W. The available experimental phase diagrams for W-Ta and W-V alloys describe the high temperature limit close to the melting point. These diagrams exhibit only the solid solution phases and show no ordered intermetallic phases that in principle should be expected to form at low temperatures.

Using *ab-initio* calculations, we compared enthalpies of mixing for large sets (~100 structures) of alloy configurations, considering several alternative ordered structures corresponding to the same chemical composition. In this way we have identified the lowest energy intermetallic compounds that are expected to dominate alloy microstructures, and hence the low temperature part of phase diagrams, for both alloys. We compared the volume relaxed configurations of alloys with those given by Vegard's law, and found that W-V alloys exhibit almost no structural relaxation. *Ab-initio* calculations also show that vanadium atoms strongly trap self-interstitial atom defects in W-V alloys, whereas Ta atoms in W-Ta alloys have very little effect on either the formation energy or thermally activated mobility of self-interstitial atom defects.

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STRESS EFFECTS ON STABILITY AND DIFFUSION OF H IN INTRINSIC W: A FIRST-PRINCIPLES STUDY

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Tungsten (W) has been chosen as one of the most promising Plasma Facing Materials (PFM) in Tokamak recently. However, W will be exposed to extremely high fluxes of hydrogen (H) isotope ions and thermal stress in Tokamak, leading to surface blistering. In our previous studies [1-3], the H behaviors in W with vacancy and other impurities such as O have been carried out by a first-principles method. A microscopic vacancy trapping mechanism for H bubble formation in W has been revealed [2]. However, effects of applied stress on the behaviors of H and thus the H bubble formation in W, though important, remain unknown.

In this paper, we have performed first-principles calculations based on density functional theory with generalized gradient approximation to investigate the stability and diffusion of H in intrinsic W under an applied stress. A three-axis stress is introduced by changing the dimension of the supercell. Both tensile and compressive stresses are taken into account. The applied stress is shown not to alter the site preference of a H atom in intrinsic W energetically. Single H atom still tends to occupy the tetrahedral interstitial sites (TIS) in comparison with octahedral interstitial sites (OIS) with 0.4 eV lower of solution energy. Further, we apply a drag method to investigate the diffusion behavior of H in intrinsic W under applied stress. The diffusion energy barrier of H atom in W is shown to decrease (increase) with the increasing tensile (compressive) stress. H thus easily diffuses into vacancy with the tensile stress. Continue investigation is in process.

FIRST-PRINCIPLES STUDY OF HYDROGEN BEHAVIOR IN V-4TI-4CR ALLOY

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Abstract: V–4Cr–4Ti alloy is considered as the most promising candidate structural material for fusion reactor due to its low induced activation, high thermal stress factor, better creep resistance, and superior mechanical performances. Hydrogen impurities derived from bombarding with the reaction plasma as well as the nuclear transmutation reaction between fast neutron and metal atoms have a considerable impact for the performance and stability of V-4Ti-4Cr alloy. To understand the microscopic mechanism, we have simulated the behaviors of H atoms inside the pure vanadium solid and V-4Ti-4Cr alloy using density functional theory and planewave pseudopotential approach. The binding energies of H atom for different interstitial sites were compared to determine the optimal trapping sites. Interaction between two interstitial H atoms was calculated and fit to a screened Coulomb potential. The diffusion path and corresponding energy barriers of H atom were computed and discussed.
FISSION-FUSION MIXED NEUTRON FIELD

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Abstract:

Fission-fusion mixed neutron fields has very important role on studying irradiation damage and the irradiation biological effects. In this paper, the physical designs about Fission-fusion mixed neutron field were introduced. The local mixed neutron fields which use the LiD and uranium target as converter material were converted from the high-intensity reactor thermal and fission fast neutron fields. The structure of the conversion target and the material of neutron spectrum adjustment were optimal designed through the MCNP code. The structure of the converter target, the neutron spectrum of the Fission-fusion mixed neutron field and the heating rate distribution were obtained.

Key words: Fission-fusion mixed neutron fields; converter target; MCNP code
FIRST-PRINCIPLES INVESTIGATION ON THE EFFECT OF CARBON ON HYDROGEN TRAPPING IN TUNGSTEN

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Tungsten (W) and W alloys are deemed as a promising candidate for plasma facing material (PFM) in a fusion reactor. It is experimentally demonstrated that extremely high fluxes of hydrogen (H) isotope ions can induce surface roughening and blistering of W, which is associated with the presence of vacancies and impurities. Carbon (C) is commonly considered as one of the most frequent impurities in W, and could influence the retention of H in W [1]. By using a first-principles method, we investigate the effect of C on H trapping in W, so that we are able to understand the surface blistering mechanism of H in W with C impurity.

In the bulk W, individual single C atom is energetically favorable sitting at the octahedral interstitial site (OIS), while individual single H prefers to occupy the tetrahedral interstitial site (TIS) [2]. When we investigate the interaction between the single C and single H in the bulk W, the computation shows that the C-H interaction is repulsive with the distance of 2.5 Å. C and W bond with a distance of ~2.2 Å, consistent with the corresponding experimental value [3]. C takes priority of bonding with W, and C and H do not attract with each other.

With the presence of the monovacancy in W, the most stable site for single C atom to be at a position is ~1.31 Å off the vacancy center close to an OIS [4]. H prefers to bind onto an isosurface of the same charge density (0.10 electron/Å³) surrounding the vacancy, a little lower than the value (0.11 electron/Å³) of the case without C atom [4]. This is should be because the presence of C induces a volume expansion of the vacancy. As shown in Fig. 1, first five H atoms occupy one-by-one the five sites surrounding the vacancy on the isosurface of the optimal charge density. The sixth H atom is shown to bond with C with the length about 1.08 Å with a CH₄-like configuration, and the isosurface of the optimal charge density for H disappears. Charge density distribution indicate the C atom is primary to bond with H in comparison with W. Average trapping energy of H in W with C is higher than that of H in W without C [4], suggesting a strong effect of C on H trapping.

References
Mobility of self-interstitial defects and small dislocation loops in Fe-Cu-Ni alloys: model alloy for RPV steels

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Reactor pressure vessel (RPV) steels are known to undergo hardening and embrittlement under neutron irradiation. This is attributed to the formation of nanometric precipitates, dislocation loops and voids. In recent years, atomistic simulations have shown to be a helpful tool to better understand the mechanisms leading to the material's degradation and to be a good supplementary tool to rationalize experiments. In particular, atomic-scale simulations allow to consider tiny details of the interaction between point defects and impurities, which are very well to known to affect significantly the evolution of microstructure. Here, we consider ternary Fe-Cu-Ni alloy as a first approximation to a model RPV steel.

In this work, we characterize the interaction of small 1D-mobile self-interstitial atom (SIA) clusters, as observed to form cascades, with Cu and Ni solutes. On the one hand, we use static simulations to characterize the energetics of interaction between SIA clusters and solutes. On the other hand, we use a recently developed “loop-drag” model, formulated by Rong et al., to estimate the mobility of dislocation loops at finite temperature. The latter model allows one to correlate the drag coefficient for the dislocation dragging the loop to the loop diffusion coefficient. Thus, we apply this model to calculate the effective mobility of SIA clusters as a function of alloy composition and temperature. The obtained results can serve as input parameters for object kinetic Monte Carlo and mean field theory models which treat 1D-migrating dislocation loops.
THE IMPORTANCE OF THE INTERACTION RADIUS BETWEEN CR AND SELF-INTERSTITIAL FE IN OBJECT KINETIC MONTE CARLO CALCULATIONS OF IRRADIATED FE-CR DILUTED ALLOYS

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Object kinetic Monte Carlo (OkMC) models allow to study the evolution of the damage created by irradiation to time scales that are comparable to those achieved experimentally. Therefore, they can be used to validate the parameters in the model through comparison with experiments. However, this validation is not trivial since a large number of parameters are necessary, including migration energies of point defects and defect clusters, binding energies of point defects to clusters, as well as the radius of interaction between defects. This is particularly cumbersome when describing an alloy, such as the Fe-Cr system of interest for fusion energy applications.

In this work we describe an object kinetic Monte Carlo model for Fe-Cr alloys in the dilute limit. The parameters used in the model come either from density function theory calculations or from empirical potentials, as obtained by different authors. This OkMC model is used to reproduce experiments performed by Abe and Kuramoto [1] of electron irradiation Fe-Cr alloys for low Cr concentrations (below 1%) and isochronal annealing. The comparison between the model and these experiments reveal that an important parameter is the capture radius between Cr atoms and self-interstitial Fe atoms. A parametric study is presented on the effect of this parameter on the simulation results.

COMPUTER SIMULATION OF RADIATION DAMAGE IN Fe-Cr ALLOY PRODUCED BY NEUTRON

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Monte Carlo method has been performed to calculate primary knock-on atome (PKA) energy spectra and PKAs’ spatial distribution in Fe-Cr alloy irradiated by neutrons. Primary damage in displacement cascades are investigated by molecular dynamics. Empirical potentials for the alloy of EAM has been constructed. The simulations are carried out for a wide range of temperature (100-600K), and PKA energy (5-20keV). The dependence of the number of Frenkel pairs and the fraction of point defects in clusters on temperature and PKA energy are obtained. The structure and properties of interstitial and vacancy clusters in Fe-Cr are discussed in the paper.

SURFACE AND GRAIN BOUNDARY SEGREGATION IN LOW Cr Fe-Cr ALLOYS: THE EFFECT OF RADIATION INDUCED VACANCIES STUDIED BY METROPOLIS MONTE CARLO SIMULATIONS

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Radiation damage may modify the segregation state and phase separation conditions in Fe-Cr alloys with compositions and temperatures of technological interest. Based on the assessment provided in a companion presentation at this conference, we use Metropolis Monte Carlo simulations to study segregation effects at surfaces and at the best stable variant of the $\Sigma=5$ (210) grain boundary, in the 5-20 at. percent range of Cr composition. The role of irradiation induced vacancies is discussed. At low Cr composition, an oscillatory segregation profile is evidenced in the vicinity of surfaces and of the $\Sigma=5$ (210) boundary. In specific conditions, Cr ordering is observed in the vicinity of the boundary. The correlation between this ordering and the occurrence of a high concentration of vacancies is discussed.
The void ordering has been observed in very different radiation environments ranging from metals to ionic crystals bombarded with energetic particles. The void ordering is often accompanied by a saturation of the void swelling with increasing irradiation dose, which makes an understanding of the underlying mechanisms to be both of scientific significance and of practical importance for nuclear engineering.

In this presentation, we compare the popular mechanisms of the void ordering based on anisotropic interstitial transport [1-4] with original mechanism based on the anisotropic energy transfer provided by self-focusing discrete breathers or quodons (energetic, mobile, highly localized lattice excitations that propagate great distances along close-packed crystal directions) [5-7]. We show that the mechanism of the void ordering is connected with radiation-induced “annealing” of selected voids, which requires special irradiation conditions. Under typical irradiation, radiation-induced driving force for the void growth prevails over that for the void annealing. We observe experimentally the radiation-induced void annealing by lowering irradiation temperature of nickel and copper samples pre-irradiated to produce voids or gas bubbles. The bulk recombination of Frenkel pairs increases with decreasing temperature resulting in suppression of production of freely migrating vacancies (the driving force of the void growth). On the other hand, the rate of radiation-induced vacancy emission from voids due to the void interaction with quodons remains essentially unchanged, which results in the void dissolution. The experimental data obtained for different metals and irradiating particles are explained by the quodon model assuming the quodon propagation length to be in the micron range, which is consistent with independent data on the irradiation-induced diffusion of interstitial ions in austenitic stainless steel [8].

VACANCIES AT TILT $\Sigma 5$ (210) AND $\Sigma 3$ (111) GRAIN BOUNDARIES IN IRON-CHROMIUM SYSTEM

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The Fe-Cr alloys serve as a model system to understand microscopic mechanism behind various processes occurring in real materials. One of such processes is the segregation/depletion of chromium at grain boundaries (GBs), which necessarily involves vacancies.

Upon irradiation, vacancies and interstitial atoms are produced and may travel through the material. Such vacancies mostly recombine with neighboring interstitial atoms, but some of vacancies may travel further and reach GBs. A number of vacancy configurations at the tilt $\Sigma 5$ (210)[001] and $\Sigma 3$ (111)[-110] GBs in iron, examined in detail in a companion presentation at this conference, are investigated. These configurations include isolated vacancies, vacancy clusters as well as various random distributions of vacancies at the studied GBs. Vacancy configurations are obtained using molecular dynamics using the state-of-the-art interatomic potentials. At very low temperatures, vacancies are stable and keep their open volume. As the temperature increases, various processes occur. In particular, vacancies may jump to other sites at the GB and/or the vacancy open volume may diminish via rearrangement of surrounding atoms. In this way it is illustrated how grain boundaries serve as a sink for vacancies. The influence of Cr atoms at GBs on the vacancy behavior is also discussed.
THE ROLE OF Y$_2$O$_3$ FOR ODS ANTI-IRRADIATION PROPERTY REVEALED BY AB INITIO CALCULATIONS

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Oxide dispersion-strengthened (ODS) ferritic steels are proposed as structural materials for future nuclear fission and fusion reactors due to their excellent mechanical properties at both room and elevated temperatures. These properties are attributed to the presence of a high density of very small oxide particles such as crystalline Y$_2$O$_3$. An addition of Ti element reduces the size of the particles. These particles are resistant to coarsening and dissolution under irradiation conditions, which result in a large number of vacancies and self-interstitial atoms and their small clusters. Among these defects, vacancies in Y$_2$O$_3$ play an important role for anti-irradiation property of ODS ferritic steels. To understand the role of vacancies, we employ *ab initio* calculation methods to study their properties, such as vacancy formation energies, vacancy-vacancy interactions and their electronic structures etc. It turns out that, for monovacancies, neutral and charged vacancies can be stable depending on the Fermi level and chemical potentials. It is found that a new electronic state appears in the middle of the Y$_2$O$_3$ band for a single O vacancy, indicating that electrons are well localized at the vacancy site. For Y single vacancy, there are two different sites in crystalline Y$_2$O$_3$, and vacancy is readily to form in the site with less effective charges. The presence of Y vacancy does not create a new state like O vacancy, but it only reduces density of states for Y. For O-O divacancies, the third nearest configuration is the most stable due to the geometrical constrain of the structure. For Y-Y divacancies, the most stable configuration is the two vacancies located at the sites with less effective charges, while two vacancies at other Y sites repel each other. For Y-O vacancies, O vacancy has a strong affinity with Y vacancy, because there exists positive and negative charge interaction between them owing to extra electrons in a neutral O vacancy and less electrons in an Y vacancy. Thus, the binding energies of Y-O vacancies become remarkable large and the formation energies of the vacancy pairs become very small. It is also observed that if Y-O vacancy pair preexists, it will attract other vacancies to form stable vacancy clusters. This mechanism makes ODS ferritic steels accommodate high vacancy concentration, suggesting that the oxide particles can act as sinks for defects to enhance anti-irradiation properties.
NUCLEATION AND GROWTH OF SELF-INTERSTITIAL ATOM CLUSTERS IN $\beta$-SiC DURING IRRADIATION

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Silicon carbide (SiC) materials are one of candidates for the blanket structural material of nuclear fusion reactors. Irradiation effects on microstructure changes in the composites has been experimentally observed, in which self-interstitial atom (SIA) loops are observed by transmission electron microscopy when irradiation temperature is greater than 600 °C. This temperature is much greater than the corresponding temperature of SIA-loop formation in metals during irradiation. Nucleation and growth of a defect cluster during irradiation is determined by the net flux of mobile defects to the cluster. The outflux of mobile defects from a cluster is determined by the binding energy of a mobile defect to the cluster. The binding energy is derived from formation energy of defect clusters; however, such formation energy in SiC materials is not clarified enough.

In the present study, formation energy of SIA-clusters in cubic silicon carbide ($\beta$-SiC) was investigated using a molecular dynamics (MD) technique. Interatomic potentials employed here for describing atomic interactions in $\beta$-SiC was Gao-Weber potential [1] that was the Brenner type function. A computational system containing an SIA-cluster in $\beta$-SiC was first relaxed at finite temperature, and was quenched to 0 K to obtain the total energy of the relaxed system [2].

The calculated formation energies of isolated silicon and carbon SIAs in $\beta$-SiC are 3.17 eV and 3.24 eV, respectively [2]. The formation energy of SIA-clusters shows an increasing function of cluster size, which is roughly in proportion to $n^1$ and $n^{1/2}$, where $n$ is the total number of SIAs in the cluster. This size dependence is very similar to the case of SIA-loops in metals. The binding energy of an SIA to an SIA-cluster in $\beta$-SiC is greater than in Fe, which may lead to the experimental fact of SIA-loop formation at high temperature. Also, the binding energy depends on the constitution ratios (Si/C) of silicon and carbon SIAs contained in a cluster.

With the obtained binding energy, the nucleation and growth process of SIA-loops in $\beta$-SiC was then investigated using a kinetic Monte Carlo (KMC) technique.

MODELING RESISTIVITY RECOVERY EXPERIMENTS WITH EVENT-BASED MONTE CARLO: BEYOND THE BINARY COLLISION APPROXIMATION

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Resistivity recovery experiments have proved very useful to probe the phenomena occurring at the atomistic scale. Indeed, after an irradiation at low temperature, a sequence of isochronal annealing sweeps in ascending order the temperature ranges where the various migration and clustering mechanisms of point defects come into play [1]. Coupled to simulations, such experiments appear to be an efficient tool to validate these mechanisms [2].

A previous numerical study on pure iron, using an event-based kinetic Monte Carlo (EKMC) code, had shown an overall good agreement with experiments [2]. However, this method is based on the binary collision approximation whose validity remains to be checked. Another EKMC method has recently been proposed, which does not rely on such an assumption [3]. We will focus on the comparison of the two codes in different experimental conditions to highlight their range of validity. A comparison with cluster dynamics, which is an efficient mean field method that provides a rigorous framework for the definition of emission rates of clusters, will also be performed at high temperature, where spatial correlations can be safely ignored.

MD STUDY ON CARBON FILM DEPOSITION

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Hydrogen-free carbon film deposition is studied through molecular dynamics (MD) simulation in view of deposition rate. MD simulation is performed for low-energy carbon particle impacts on carbon surfaces at room temperature. Deposited particles are considered C and C\textsubscript{2} with deposition energy up to $E = 50$ eV per carbon atom. Deposited surface is set amorphous, and low-index surfaces are considered to compare. In this MD simulation, the C-C force is described by the analytical bond-order potential and the Moliere potential for an equilibrium range and a short range, respectively.

For low-index surfaces, three characteristic regions are found on the deposition state such as shallow trapping in $E < 20$ eV, deep trapping in $E > 30$eV about normal incidence, and reflection in $E > 30$eV about grazing incidence. However, for the amorphous surface, high-ratio of shallow trapping is found at all incident angle. Thus the deposition rate is mainly determined by the sputtering yield. Table 1 shows the deposition rate at normal incidence with other experimental and MD results. The present result is reasonable, considering the low-deposition energy compared with other experiment and MD calculation.

\begin{table}[h]
\centering
\begin{tabular}{lcccc}
\hline
 & Experiment [1] & TBMD [2] & This MD \\
\hline
Deposition energy & 600eV & 300eV & 100eV & 30-50eV \\
\hline
Self-sputtering & 0.74-0.79 & 0.47-0.58 & 0.43 & 0.23-0.33 \\
Deposition rate & 0.26-0.21 & 0.53-0.42 & 0.57 & 0.77-0.67 \\
\hline
\end{tabular}
\caption{Deposition rates on hydrogen-free carbon film formation}
\end{table}

MOLECULAR DYNAMICS SIMULATIONS OF EFFECTS OF HIGH ELECTRIC FIELDS ON METAL NANOTIPS

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Strong electric fields above metal surfaces in high vacuum lead to electric arcs. This phenomenon is utilized in Metal Vapor Vacuum Arc (MEVVA) ion sources, used in e.g. ion implantation, thin film deposition and particle accelerators, due to the pure ion beam and high current that is produced. In other cases, the arcs can, however, damage sensitive parts, such as particle accelerating structures, lowering their performance. It is, therefore, of great importance to gain a good understanding of the conditions that lead up to arcing.

It is believed that atoms that evaporate from small tips on the cathode build a plasma, causing arcing. Using Molecular Dynamics simulations we have studied how tip geometry, field enhanced evaporation[1], field emission and electronic heat conduction affect the evaporation rate of atoms from the tip. We implemented explicitly these processes by solving the 1D heat equation, which accounts for the resistive heating and the thermal conduction by electrons. Additionally, our model also accounts for black body radiation from the tip. Thus we broadened the applicability of the MD method to include electronic effects.

Because the tips we studied were of the same order of magnitude as the mean free path of the electrons moving inside them, size effects were also considered. Both the electrical resistivity and thermal conductivity are strongly affected by the tip diameter[2].

Using the new code we simulated a small copper tip on a copper surface under a high electric field. Simulations were performed with both purely thermal evaporation and field enhanced evaporation enabled, with only field enhanced evaporation enabled (resistive heating not included), and with only thermal evaporation enabled (no charges on atoms added).

The simulations show that the tip under the electric field must be sufficiently tall to reach melting temperature, at which point atoms evaporate more easily. A too short tip leads to highly efficient heat transportation out of the tip, while a too wide tip leads to insufficient resistive heating to raise the temperature of the tip up to its melting point. Additionally, we have shown that for accurate estimation of the evaporation rate of neutral atoms, both field enhanced evaporation and thermal evaporation must be considered.


Fig. 1: Atoms evaporating from tip
GENETIC OPTIMIZATION OF NOBLE GAS CLUSTERS DOPED WITH METAL IONS

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Genetic algorithm is the optimization technique based on the idea of improving the adaptation of individuals in population. Its usefulness in solving the problems devoted to the determination of atomic clusters shape has been confirmed in numerous approaches [1-3]. In the proposed paper we show the results of calculations performed in order to optimize the configurational energy of noble gas clusters doped with single as well as greater number of alkali metal ions. Such a structures are characterized by interesting electronic [4] and structural properties. There were also reported interesting effects accompanying the collisions between both types of atoms.

In our paper we present structural considerations concerning the energies and topology of studied clusters following the simple forms of two-body potentials. We discuss the existence of so called magic numbers and the appearance of caging of alkali metal ions.

FREE VOLUME EVOLUTION IN 50 MeV Li$^{3+}$ ION IRRADIATED POLYMERS STUDIED BY POSITRON ANNIHILATION LIFETIME

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ABSTRACT

Free volume properties of polymeric materials change with Swift Heavy Ion (SHI) irradiation. The change depends on the polymer and ion, its energy and fluence. Free volume is found to have strong correlation with the macroscopic properties of the polymer. Positron Annihilation Lifetime Spectroscopy (PALS) has recently emerged as a unique non-destructive and non-interfering nano-probe, capable of measuring the free volume hole size in polymers with high detection efficiency [1, 2]. Polyamide nylon-6 (PN-6) and polyethersulphone (PES) films of thickness of 250 lm were irradiated with Li$^{3+}$ ions of energy 50 MeV from 15 UD Pelletron accelerator at Inter University Accelerator Centre (IUAC), New Delhi, India. PN-6 films were irradiated to the fluences of $10^{10}$, $10^{11}$, $10^{12}$ and $10^{13}$ ions/cm$^2$ whereas PES films were irradiated to the fluences of $10^{11}$, $10^{12}$, $10^{13}$ and $10^{14}$ ions/cm$^2$. Characterization of the effect of ion irradiation on free volume has been done by PALS. The average free volume and fractional free volume obtained from long lived component, attributed to ortho-positronium (o-Ps) lifetime, are found to decrease with the fluence in both the cases. With increasing fluence, scissioned segments cross-link randomly, resulting in a decrease of average free volume due to overlapping of tracks. Results will be discussed.

References:

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PHYSICAL AND CHEMICAL RESPONSE OF 145 MeV Ne$^{+6}$ ION IRRADIATED POLYMETHYL METHACRYLATE (PMMA) POLYMER

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Abstract

Characterization of ion induced modifications in the physical, chemical and structural properties of Polymethylmethacrylate (PMMA) polymer due to 145 MeV Ne$^{+6}$ ion irradiation has been carried out by FTIR, UV-Visible, Differential Scanning Calorimetry (DSC) and X-ray Diffraction. Heavy ion irradiation was carried out under a vacuum of $\sim 10^{-6}$ torr at the Variable Energy Cyclotron Centre, Kolkata, India using a low beam current ($\sim 15$ nA). Ion fluences of $10^{10}$, $10^{11}$, $10^{12}$, $10^{13}$ ions/cm$^2$ were used. The optical band gap ($E_g$), calculated from the absorption edge of the UV spectra of these films in 200-800 nm region varied from 2.167 eV to 1.512 eV for virgin and irradiated samples. In FTIR spectra, appreciable changes have been observed after irradiation, indicating the molecular fragmentation, cross-linking, formation of unsaturated group and free radicals. DSC thermograms give information about the thermal stability and type of thermal reactions (exothermic/endothermic) on the application of heat to the polymer. XRD analyses show slight shift of peak position and significant changes in peak intensity. XRD results show a decrease of $\sim 4.12\%$ in crystallite size of irradiated sample at the higher fluence of $10^{12}$ ions/cm$^2$. 
RIETVELD COMPUTER SIMULATION OF NANOSTRUCTURAL LaMnO₃ PEROVSKITE MANGANITE BY X-RAY BEAM SCATTERING

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Abstract

The nanostructural LaMnO₃ perovskite manganite investigated by X-ray beam diffraction (XRD). Our sample have been synthesized by the amorphous heteronuclear complexing method at 800 °C temperature. X-ray beam diffraction analysis using Rietveld simulation show that our sample is single phase and crystallize in the rhombohedral distorted perovskite structure with $R\bar{3}c$ space group and with lattice parameters of $a = b = 0.550$ and $c = 1.334\text{nm}$. It was established considerable distortion of oxygen atom in the rhombohedral structure from own initial positions $4b$. Our results indicate that oxygen excess parameter for LaMnO₃ is 0.29.

Keywords: perovskite, crystal structure, x-ray diffraction, oxygen vacancies, Rietveld simulation method
ESTIMATION OF THE DETECTION EFFICIENCY FOR CR-39 NTDs AND THE CALIBRATION FACTOR FOR DIFFERENT DOSIMETER FOR RADON AND THORON GAS

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The detection efficiency of CR-39 for alpha particles and their effects on the calibration factor (K) for radon and thorn has been studied, the results showed that this factor relatively depend on the detector efficiency, it is increasing exponentially with increasing of the efficiency of CR-39, TRACK-TEST program was used for estimate the optimum detection efficiency for track registration of CR-39 and it was equal to 80.3%.

As well as, the calibration factor (K) of radon and thoron for the optimum dimension (diameter=6cm, height=7cm & cylindrical shapes) of the dosemeters have been estimated and as shown in Fig.1. So it is necessary to take the calibration factor and the detector efficiency it into account for the detection of radon and thoron gas

Fig.1 Optimum dimension of the radon and thoron dosimeters

References:
MASS DEPENDENCE OF SPUTTERING CHARACTERISTICS FOR A NUMBER OF METALS WITH DIFFERENT PROPERTIES

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Molecular dynamic simulation has been used to study how the sputtering characteristics of metal polycrystals are dependent on the mass $m_1$ of bombarding ions of low energy $E_0$. This is a continuation of our investigations of anomalous mass dependence of target sputtering by low-energy ions [1] with the model presented in [2]. The influence of target parameters on mass dependence of sputtering has been calculated for Al, Ba, Ce and Au, which we were not previously studied in detail. These metals have very different values of density $\rho$, the lattice constant $d$, and the surface bonding energy $E_b$ (see tab.1) – the parameters that define the sputtering process [3].

The targets were bombarded by Li, B, N, Al, Ar, Ni, Ga, Kr, Xe ions with $E_0$ from 200 to 2000 eV. Mass dependences of sputtering yield $Y$, depth of origin $\bar{x}_0$, mean energy $\bar{E}_1$, and number of generations $L$ of sputtered particles have been shown to be non-monotonic, especially for low $E_0$ (Figs.1,2).

It is interesting that the curves $Y(m_1)$ for Ba, Ce, and Au – metals with very different properties – are practically the same not just qualitatively but also quantitatively (small difference are seen only for low $E_0$). In the same time the functions $L(m_1)$ are different for these metals. Indeed, for Ba and Ce there is a monotonic rise of $L$ with $m_1$, however for Au a minimum of the curve $L(m_1)$ is observed. The $\bar{x}_0$ ($m_1$) dependencies for all the studied metals drop with the increase of $m_1$; the maximal value of $\bar{x}_0$ is observed for Ce (50 Å for $E_0=2$ keV).

In summary the features of sputtering characteristics for the studied metals are discussed. The main reason for non-usual behaviour of Au sputtering is explained by the highest density and low binding energy of this metal as compared to the other metals in the study.

<table>
<thead>
<tr>
<th>Table 1.</th>
<th>Al</th>
<th>Ba</th>
<th>Ce</th>
<th>Au</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$, g/cm$^3$</td>
<td>2.7</td>
<td>3.76</td>
<td>6.75</td>
<td>19.3</td>
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<tr>
<td>$d$, Å</td>
<td>4.05</td>
<td>5.10</td>
<td>5.16</td>
<td>4.08</td>
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<tr>
<td>$E_b$ eV</td>
<td>3.34</td>
<td>1.86</td>
<td>4.77</td>
<td>3.81</td>
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</table>

Fig.1. Sputtering yield versus mass of bombarding ions with $E_0$ of 200, 300, 500, 1000, 1500, 2000 eV rising from the bottom curve to the top one.

Fig.2 Number of generations $L$ leading to sputtering ($E_0$ are the same as in Fig.1).

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Notes
Author Index
# Author Index

**A**

Achkeev, A. A. ................................................. 107  
Agullo-Lopez, F. ............................................. 121  
Akkerman, A. .................................................. 120  
Albe, Karsten .................................................. 67  
Ali, S. A. .......................................................... 144  
Al-Motasem, A. T. ........................................... 93  
Anders, Christian ............................................. 104  
Angibaud, L. .................................................... 97  
Aoki, Takaaki ................................................... 37  
Astapenko, V. A. ............................................. 109, 110  
Aziz, Michael J. .............................................. 60

**B**

Bai, Xian-Ming ................................................ 78  
Baluc, N. L. ..................................................... 126  
Barak, J. .......................................................... 120  
Batemberel, G. ............................................... 145  
Bazzanella, Nicola .......................................... 112  
Becquart, C. S. ............................................... 72, 88  
Berepazki, V. V. ............................................ 109  
Bergner, F. ...................................................... 93  
Bertolus, Marjorie .......................................... 124  
Betz, G. .......................................................... 100, 101  
Bhatt, Poonam ............................................... 143  
Blackwell, S. ................................................... 85  
Bocquier, J.-L. ................................................ 91  
Bogaerts, A. .................................................... 116  
Bonny, G. ......................................................... 131  
Bousis, Christos ............................................ 115  
Boyle, K. P. ...................................................... 92  
Bracht, hartmut ............................................... 59  
Briquet, L. ....................................................... 61, 97  
Brutzel, Laurent Van ....................................... 75  
Budil, Matthias ............................................... 105  
Bulatov, V. V. .................................................. 139

**C**

Calliari, Lucia ............................................... 111  
Caro, A. .......................................................... 70  
Caro, M. .......................................................... 70  
Castin, N. ......................................................... 83, 131  
Caturla, M. J. .................................................. 79, 91, 121, 122, 132  
Chandraal, Sh. .............................................. 145  
Cui, Xiaojun ................................................... 65  
Czerwiński, Bartłomiej ................................. 102, 103

**D**

Dapor, Maurizio ........................................... 53, 111, 112  
Daraszewicz, Szymon ..................................... 48  
Das, D. ............................................................ 143  
Davila, L. P. ................................................... 121  
De, Udayan .................................................... 144  
DeBacker, A. ................................................... 72  
Delcorte, Arnaud ............................................ 34, 40  
Deng, Huiqiu .................................................. 65  
Derrien, Thibault J. Y. .................................... 114  
Devanathan, Ram ......................................... 68, 118  
Diaz, D. ........................................................... 122  
Dinnebier, R. E. ............................................. 145  
Djurabekova, Flyura ..................................... 49, 63, 119, 141  
Domain, C. ................................................... 72, 88  
Donev, A. ........................................................ 139  
Dorado, Boris ................................................ 124  
Doyama, Masao ............................................. 41  
Dubinski, V. I. ............................................... 135  
Dudarev, S. L. ............................................... 126  
Duffy, Dorothy .............................................. 45, 48  
Duin, Adi C. T. van ....................................... 29  
Dunn, Alastair ............................................... 45  
Duvendeck, A. ............................................... 52, 113  
Dytlewska, N. ............................................... 73  
Dzhurakhalov, A. A. .................................... 99, 116

**E**

Emfietzoglou, Dimitris .................................. 115  
Erhart, P. ......................................................... 70  
Ewing, Rodney C. ......................................... 68

**F**

Facsko, S. ....................................................... 87  
Finnis, M. W. ............................................... 47  
Foulkes, W. M. C. ......................................... 47  
Freyss, Michel ............................................... 124  
Fu, Chu Chun ............................................... 79, 90, 91  
Fukahori, Tokio ........................................... 77  
Fukoshige, Akinori ....................................... 98

**G**

Galbaatar, T. ............................................... 145  
Gamez, B. ...................................................... 132  
Gamez, L. ...................................................... 132  
Gao, F. ........................................................... 31, 82
<table>
<thead>
<tr>
<th>Author Index</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Garrison, Barbara J.</strong> 32, 34, 38, 39, 54, 56, 102, 103</td>
</tr>
<tr>
<td>Gerolf, Ziegenhain ........................................... 104</td>
</tr>
<tr>
<td>Gianlanello, Stefano ........................................... 112</td>
</tr>
<tr>
<td>Grigorjev, D. V. .................................................. 106</td>
</tr>
<tr>
<td>Guglya, A. G. .................................................... 135</td>
</tr>
<tr>
<td>Gumus, Hasan .................................................... 108</td>
</tr>
<tr>
<td>Gwizdala, Tomasz M. ........................................... 142</td>
</tr>
<tr>
<td><strong>H</strong></td>
</tr>
<tr>
<td>Hadjidoukas, Panagiotis ....................................... 115</td>
</tr>
<tr>
<td>Hanke, S .......................................................... 52, 113</td>
</tr>
<tr>
<td>Harjunmaa, Ari ................................................... 67</td>
</tr>
<tr>
<td>Hashimoto, Naoyuki ............................................ 77</td>
</tr>
<tr>
<td>Hashimoto, Satoshi ............................................. 77</td>
</tr>
<tr>
<td>Heinig, Karl-Heinz ............................................... 66, 87</td>
</tr>
<tr>
<td>Hernandez-Mayoral, M. ........................................ 122</td>
</tr>
<tr>
<td>Hnatowicz, V. .................................................... 107</td>
</tr>
<tr>
<td>Hoagland, Richard G. ........................................... 78</td>
</tr>
<tr>
<td>Hobler, Gerhard .................................................. 46, 105</td>
</tr>
<tr>
<td>Holmstrom, E. ..................................................... 64</td>
</tr>
<tr>
<td>Horsfield, A. P. ................................................... 47</td>
</tr>
<tr>
<td>Hou, M. ............................................................. 72, 80, 88, 134, 136</td>
</tr>
<tr>
<td>Hu, Wangyu ....................................................... 31, 65</td>
</tr>
<tr>
<td>Hyakutake, T. ..................................................... 140</td>
</tr>
<tr>
<td>I</td>
</tr>
<tr>
<td>Ilyin, A. M. ....................................................... 123</td>
</tr>
<tr>
<td>Ishino, Shiori ...................................................... 77</td>
</tr>
<tr>
<td>Ismail, Asaad H. .................................................. 146</td>
</tr>
<tr>
<td>Itina, Tatiana E. .................................................. 114</td>
</tr>
<tr>
<td>Ito, Takahiro ....................................................... 77</td>
</tr>
<tr>
<td>Iwase, Akihiro ..................................................... 89</td>
</tr>
<tr>
<td>Iwase, Hiroshi ...................................................... 77</td>
</tr>
<tr>
<td>Iwata, Shuichi ..................................................... 89</td>
</tr>
<tr>
<td>Izhnin, I. I. ........................................................ 106</td>
</tr>
<tr>
<td>J</td>
</tr>
<tr>
<td>Jafaar, M. S. ....................................................... 146</td>
</tr>
<tr>
<td>Jansson, V. ........................................................ 76, 131</td>
</tr>
<tr>
<td>Jiang, C. ........................................................... 74</td>
</tr>
<tr>
<td>Joly, L. ............................................................. 91</td>
</tr>
<tr>
<td>Jourdan, T. ........................................................ 91, 139</td>
</tr>
<tr>
<td>K</td>
</tr>
<tr>
<td>Kabadai, Onder .................................................... 108</td>
</tr>
<tr>
<td>Kaneko, Yoshihisa ............................................... 77</td>
</tr>
<tr>
<td>Kaneta, Yasunori .................................................. 89</td>
</tr>
<tr>
<td>Karim, Eman Tahir Abdul ....................................... 55</td>
</tr>
<tr>
<td>Kawai, Masayoshi ............................................... 77</td>
</tr>
<tr>
<td>Matsuo, Jiro ....................................................... 37</td>
</tr>
</tbody>
</table>
Author Index

Menshikov, L. I. ........................................ 109
Menshikov, P. L. ........................................ 109
Michely, Thomas .................................... 117
Miller, R. E. ........................................... 92
MIotello, Antonio .................................... 112
Mody, Jaydeep D. .................................... 35, 50
Moller, W. ............................................. 87
Momota, Sadao ....................................... 98
Mookerjee, S. ......................................... 49
Moreira, Pedro A. F. P. .............................. 118
Morishita, Kazunori ................................ 69, 138
Mosunov, A. S. ....................................... 147
Mulroue, Jack ........................................ 48
Munkhbaatar, P. ...................................... 145
Muramoto, T. .......................................... 140
Murat, M. .............................................. 120
Muzyk, M. ............................................ 126
N
Nangia, Shivangi .................................... 56
Nastasi, Michael ..................................... 78
Nguyen-Manh, D. .................................... 126
Nikjoo, Hooshang ................................... 115
Nishida, M. ............................................ 140
Nordlund, Kai ........................................ 49, 60, 63, 64, 67, 119, 141
Norris, Scott A. ...................................... 60
Nozaki, T. ............................................. 41
Numazawa, Satoshi ................................. 66
O
Oda, Takuji ........................................... 84
Olivares, J. ............................................ 121
Ossowski, T. .......................................... 80, 134, 136
Ou, Y. D. ................................................ 137
P
Page, J. le ............................................ 47
Pakrinen, Olli ......................................... 49, 119
Paruch, Robert ...................................... 38, 102, 103
Parvainen, Stefan ................................... 141
Pathak, Anand ....................................... 115
Perlado, J. M. ......................................... 122, 132
Philipp, P. .............................................. 61, 97
Philipe G 150cia ....................................... 75
Posselt, M. ............................................ 30, 93
Postawa, Zbigniew .................................. 38, 102, 103
Prasad, Rajendra .................................... 143, 144
Q
Qian, D. Z. ............................................ 133
Qi-jie, Feng .......................................... 129
Qin, Ying ............................................. 128
R
Race, C. P. ........................................... 47
Rhamezov, S. E. ................................... 99
Rasulov, A. X. ....................................... 99
Redinger, Alex ...................................... 117
Restrepo, Oscar A ................................ 40
Rivera, A. ........................................... 121
Robinson, M. ...................................... 125
Rosandi, Yudi ....................................... 42, 117
Roy, A. ............................................... 49
Run-dong, Li ......................................... 129
Russo Jr., Michael F. ................................ 29
Rzeznik, Lukasz ................................. 38, 102, 103
S
Sabathier, Catherine .............................. 75
Sadigh, B. ........................................... 70
Samela, Juha ......................................... 60
Sangaa, D. ........................................... 145
Sarkar, U. ............................................ 72
Sarnet, Thierry ..................................... 114
Satake, Shin-ichi ................................... 98
Scarduelli, Giorgina ................................. 111
Scott, Chris .......................................... 43
Seki, Toshio .......................................... 37
Sentis, Marc ......................................... 114
Shabib, Ishraq ....................................... 92
Shibahara, Masahiko ................................ 98
Shimakawa, Satoshi ............................... 77
Shimizu, Futoshi ................................... 77
Shinya, Tomohiro .................................. 36
Shu, Xiaolin ......................................... 31
Shulga, V. I. .......................................... 100
Sickafus, K. E. ..................................... 74
Singh, F. ............................................. 143, 144
Singh, Paramjit ................................. 143, 144
Smith, Roger ......................................... 43, 85, 86, 125
Sonakwade, R. G. ................................ 143
Sonakwade, R. G. ............................... 144
Souidi, A. ........................................... 88
Soulairol, R. ......................................... 90
Stanek, C. R. ......................................... 74
Steede, J. W. ......................................... 58
Stelmakh, V. G. ................................... 99
Stoller, R. E. ......................................... 88
Storr, M. T. .......................................... 125
Stukowski, Alexander ............................. 67, 70
<table>
<thead>
<tr>
<th>Author</th>
<th>Index Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sule, P</td>
<td>44</td>
</tr>
<tr>
<td>Sutton, A. P</td>
<td>47</td>
</tr>
<tr>
<td>Syshchenko, V. V</td>
<td>110</td>
</tr>
<tr>
<td>Tagirov, L. R</td>
<td>107</td>
</tr>
<tr>
<td>Talipov, N. H</td>
<td>106</td>
</tr>
<tr>
<td>Tanaka, Satoru</td>
<td>84</td>
</tr>
<tr>
<td>Taniguchi, Jun</td>
<td>98</td>
</tr>
<tr>
<td>Tarnovsky, A. I</td>
<td>110</td>
</tr>
<tr>
<td>Terentyev, D</td>
<td>76, 131, 132</td>
</tr>
<tr>
<td>Thomas, Derek A</td>
<td>57</td>
</tr>
<tr>
<td>Toikka, L</td>
<td>64</td>
</tr>
<tr>
<td>Toniutti, Laura</td>
<td>112</td>
</tr>
<tr>
<td>Torres, Remi</td>
<td>114</td>
</tr>
<tr>
<td>Toulemonde, Marcel</td>
<td>49, 68</td>
</tr>
<tr>
<td>Tsuchihira, Hiroki</td>
<td>84</td>
</tr>
<tr>
<td>Uberuaga, Blas P</td>
<td>74, 78</td>
</tr>
<tr>
<td>Urbassek, Herbert M</td>
<td>42, 104, 117</td>
</tr>
<tr>
<td>Vernon, L. J</td>
<td>85</td>
</tr>
<tr>
<td>Victoria, M</td>
<td>122</td>
</tr>
<tr>
<td>Virk, H. S</td>
<td>144</td>
</tr>
<tr>
<td>Voitsekhovskii, A. V</td>
<td>106</td>
</tr>
<tr>
<td>Voter, Arthur F</td>
<td>78</td>
</tr>
<tr>
<td>Wang, Liang</td>
<td>65</td>
</tr>
<tr>
<td>Wang, Tianmin</td>
<td>31, 127</td>
</tr>
<tr>
<td>Watanabe, Y</td>
<td>138</td>
</tr>
<tr>
<td>Watanabe, Yoshiyuki</td>
<td>69</td>
</tr>
<tr>
<td>Watanabe, Yukinobu</td>
<td>77</td>
</tr>
<tr>
<td>Webb, Roger P</td>
<td>35, 50</td>
</tr>
<tr>
<td>Weber, William J</td>
<td>68, 82, 118</td>
</tr>
<tr>
<td>Weidtmann, B</td>
<td>52, 113</td>
</tr>
<tr>
<td>Wen, Bin</td>
<td>128</td>
</tr>
<tr>
<td>Wendelen, W</td>
<td>116</td>
</tr>
<tr>
<td>Willaime, F</td>
<td>91</td>
</tr>
<tr>
<td>Winograd, Nicholas</td>
<td>33</td>
</tr>
<tr>
<td>Wirtz, T</td>
<td>61, 97</td>
</tr>
<tr>
<td>Wu, Chengping</td>
<td>55, 57</td>
</tr>
<tr>
<td>Wucher, A</td>
<td>51, 52, 113</td>
</tr>
<tr>
<td>Xiao, H. Y</td>
<td>82</td>
</tr>
<tr>
<td>Xin, X. K</td>
<td>81</td>
</tr>
<tr>
<td>Yadgarov, I. D</td>
<td>99</td>
</tr>
<tr>
<td>Yamaguchi, Yasutaka</td>
<td>36</td>
</tr>
<tr>
<td>Yamamoto, Yasunori</td>
<td>69, 138</td>
</tr>
<tr>
<td>Yamashina, Shun</td>
<td>98</td>
</tr>
<tr>
<td>Yamazaki, Y</td>
<td>62</td>
</tr>
<tr>
<td>Yang, Xiyuan</td>
<td>65</td>
</tr>
<tr>
<td>Yamasato, H</td>
<td>36</td>
</tr>
<tr>
<td>Yermolenko, O. A</td>
<td>100, 101</td>
</tr>
<tr>
<td>Yong-jun, Deng</td>
<td>129</td>
</tr>
<tr>
<td>Yong-kang, Liu</td>
<td>129</td>
</tr>
<tr>
<td>Yoshiie, Toshimasa</td>
<td>77</td>
</tr>
<tr>
<td>Yoshimatsu, Junichi</td>
<td>69</td>
</tr>
<tr>
<td>Yu, Jianguo</td>
<td>118</td>
</tr>
<tr>
<td>Yurasova, V. E</td>
<td>147</td>
</tr>
<tr>
<td>Zeman, A</td>
<td>73</td>
</tr>
<tr>
<td>Zhang, Jiaying</td>
<td>68</td>
</tr>
<tr>
<td>Zhang, Jijun</td>
<td>128</td>
</tr>
<tr>
<td>Zhang, Pengbo</td>
<td>128</td>
</tr>
<tr>
<td>Zhang, Ying</td>
<td>71, 127, 130</td>
</tr>
<tr>
<td>Zhibin, Lin</td>
<td>55</td>
</tr>
<tr>
<td>Zhigilei, Leonid V</td>
<td>55, 57</td>
</tr>
<tr>
<td>Zhou, Hong-Bo</td>
<td>71, 127, 130</td>
</tr>
<tr>
<td>Zhou, W</td>
<td>133</td>
</tr>
<tr>
<td>Zhu, Yongfa</td>
<td>145</td>
</tr>
<tr>
<td>Zhurkin, E. E</td>
<td>80, 134, 136</td>
</tr>
<tr>
<td>Zykova, E. Yu</td>
<td>147</td>
</tr>
</tbody>
</table>
# COSRES-2010 Programme Overview

<table>
<thead>
<tr>
<th>Sunday, 18 July</th>
<th>Monday, 19 July</th>
<th>Tuesday, 20 July</th>
<th>Wednesday, 21 July</th>
<th>Thursday, 22 July</th>
<th>Friday, 23 July</th>
</tr>
</thead>
<tbody>
<tr>
<td>08:00 Registration</td>
<td>08:00 Registration</td>
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<tr>
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<tr>
<td><strong>Chair: Nordlund</strong></td>
<td><strong>Chair: Gao</strong></td>
<td><strong>Chair: Webb/Sigmund</strong></td>
<td><strong>Chair: Caturla</strong></td>
<td><strong>Chair: Yoshiie</strong></td>
<td></td>
</tr>
<tr>
<td>09:00 I1 Russo</td>
<td>09:00 I3 Foulkes</td>
<td>09:00 I7 Yamazaki</td>
<td>09:00 I9 Morishita</td>
<td>09:00 I12 Kenny</td>
<td></td>
</tr>
<tr>
<td>09:40 O1 Posselt</td>
<td>09:40 O17 Duffy</td>
<td>10:00 O18 Mookarjee</td>
<td>10:00 O33 Caro</td>
<td>09:40 O46 Smith</td>
<td></td>
</tr>
<tr>
<td>10:00 O2 Shu</td>
<td>10:00 O18 Mookarjee</td>
<td>10:10 I8 Djurabekova</td>
<td>10:00 O34 Lu</td>
<td>10:00 O47 Liedke</td>
<td></td>
</tr>
<tr>
<td>10:40-11:00 Coffee</td>
<td>10:40-11:00 Coffee</td>
<td>10:55-11:20 Coffee</td>
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</tr>
<tr>
<td><strong>Chair: Urbassek</strong></td>
<td><strong>Chair: Winograd</strong></td>
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<td><strong>Chair: Smith</strong></td>
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</tr>
<tr>
<td>11:00 I2 Winograd</td>
<td>11:00 I4 Wucher</td>
<td>11:20 O28 Holmström</td>
<td>11:00 O36 Zeman</td>
<td>11:00 O49 Kaneta</td>
<td></td>
</tr>
<tr>
<td>11:40 O4 Delcorte</td>
<td>11:40 O20 Duvenbeck</td>
<td>11:40 O29 Hu</td>
<td>11:20 O37 Uberuaga</td>
<td>11:20 O50 Fu</td>
<td></td>
</tr>
<tr>
<td>12:00 O5 Mody</td>
<td>12:00 O21 Dapor</td>
<td>12:00 O30 Numazawa</td>
<td>11:40 O38 Martin</td>
<td>11:40 O51 Jourdan</td>
<td></td>
</tr>
<tr>
<td>12:20 O6 Yamaguchi</td>
<td>12:20 O22 Garrison</td>
<td>12:20 O31 Harjumaa</td>
<td>12:00 O39 Janssone</td>
<td>12:00 O52 Boyle</td>
<td></td>
</tr>
<tr>
<td>12:40 Lunch</td>
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<td>12:00 O40 Yoshiie</td>
<td>12:20 O53 Al-Motasem</td>
<td></td>
</tr>
<tr>
<td><strong>Chair: Delcote</strong></td>
<td><strong>Chair: Garrison</strong></td>
<td><strong>Chair: Zurek</strong></td>
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<td><strong>Chair: Smith</strong></td>
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</tr>
<tr>
<td>14:25 O7 Aoki</td>
<td>14:25 I5 Zhigilei</td>
<td>14:25 I10 Bai</td>
<td>14:25 I10 Bai</td>
<td>13:00 Lunch</td>
<td></td>
</tr>
<tr>
<td>14:45 O8 Rzeznik</td>
<td>15:05 O23 Nangia</td>
<td>15:05 O41 Caturla</td>
<td>14:00 Adjourn</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15:25 O10 Restrepo</td>
<td>15:45 O25 Steeds</td>
<td>15:45 O43 Lai</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15:45 O11 Doyama</td>
<td></td>
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<tr>
<td>16:05-16:30 Coffee</td>
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<td>16:15 Conference outing to Wieliczka Salt Mine</td>
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<td>13:00 Lunch</td>
<td></td>
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<tr>
<td><strong>Chair: Aoki</strong></td>
<td><strong>Chair: Posselt</strong></td>
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</tr>
<tr>
<td>16:30 O12 Rosandi</td>
<td>16:30 I6 Bracht</td>
<td>16:30 I11 Gao</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>16:50 O13 Scott</td>
<td>17:10 O26 Samela</td>
<td>17:10 O44 Castin</td>
<td>17:00 Lunch</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17:10 O14 Süle</td>
<td>17:30 O27 Philipp</td>
<td>17:30 O45 Tsuchihira</td>
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<td></td>
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</tr>
<tr>
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<td></td>
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</tr>
<tr>
<td>18:00-20:00 Registration</td>
<td>18:00-20:00 Poster Session I</td>
<td>18:00-20:00 Registration</td>
<td>18:00-20:00 Registration</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19:00-21:00 Welcome reception</td>
<td>18:00-20:00 Poster Session I</td>
<td>19:00 Conference dinner at Wieliczka Salt Mine</td>
<td>17:50-19:50 Poster Session II</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>20:00 Concert</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>