

Symposium 6: Multiscale modeling of radiation effects in materials

Organizers: Pascal Bellon, Fei Gao, Syo Matsumura, Roger Stoller

Oral Presentations

Blue: Invited talk (30 minutes)

Black: Contributed talk (20 minutes)

Green: Posters presentation

Monday Afternoon -- Joint session with symposium 9

Dane Morgan, Julie Tucker, Todd Allen, Ab-initio Based Modeling of Diffusion and Radiation Induced Segregation in Ni-Fe-Cr alloys (S-6)

Alexander Barashev, Interaction of interstitial clusters with solute atoms in ferritic alloys and its consequence for microstructural development under neutron irradiation (S-6)

Christophe Domain, Pär Olsson, Edwige Aublant, Raoul Ngayam Happy, Charlotte Becquart, An ab initio based AKMC model of ferritic Fe alloys under irradiation (S-6)

Michael Jenkins, Zhongwen Yao, Mercedes Hernandez-Mayoral, Mark Kirk, Dynamic observations of heavy-ion damage in Fe and Fe-Cr alloys (S-9)

Monday Afternoon (2)

Alfredo Caro, Paul Erhart, Babak Sadigh, Giovanni Bonny, Lorenzo Malerba, Magdalena Caro, The challenge to bridge scales in computational modeling Fe alloys.

Kai Nordlund, Tommi Järvi, Antti Kuronen, Ion irradiation of nanocrystals.

Arnoldo Badillo, Robert Averback, Pascal Bellon: Microstructural evolution of binary alloys under irradiation.

Tuesday Afternoon

Alain Chartier, Tomokazu Yamamoto, Kazuhiro Yasuda, Constantin Meis, Kenichi Shiiyama, Syo Matsumura, Molecular dynamics simulation of irradiation induced phase transition in MgAl₂O₄

Ying Chen, Hua-Yun Geng, Misako Iwasawa, Yasunori Kaneta, Toshiharu Ohnuma, Motoyasu Kinoshita, First principles modeling of defects behavior in UO₂ and CeO₂

Mikhail Lavrentiev, Duc Nguyen-Manh, Sergei Dudarev, Magnetic Cluster Expansion Study of Magnetism and Thermodynamic Properties of Iron and Iron-Chromium Alloy.

Duc Nguyen-Manh, Systematic study of interactions between irradiated defects and impurities in bcc transition metals

Tuesday Afternoon (2) -- Joint session with symposium 9

C A English, M L Jenkins, Molecular ion irradiations of molybdenum (S-9)

David Stewart, Yuri Osetsky, Roger Stoller, Stanislav Golubov, Tatiana Seletskaya, Paul Kamenski, Atomistic studies of properties of helium in BCC iron (S-6)

Howard Heinisch, Atomic-scale Modeling of Helium Atoms and Vacancies in Dislocations in alpha-Iron (S-9)

Fei Gao, Atomic-Level Modeling of Migration of Vacancies, He Interstitials, and Nucleation of He-V clusters at Grain Boundaries in alpha-Fe (S-9)

Rick Kurtz, Howard Heinisch, Fei Gao, Interaction of He_nV_m Clusters with Coherent and Semi-Coherent Fe/Cu Interfaces (S-6)

Chung H Woo, Resistance to Fast Dislocation Motion (S-9)

Enrique Martinez, **Jaime Marian**, Athanasios Arsenlis, Maximo Victoria, Hyon-Jee Lee, Brian Wirth, Combined Atomistic and Dislocation Dynamics Modeling of Dislocation-SFT Interactions in Cu (S-6)

Wednesday Afternoon

M-C Marinica and **François Willaime**, Multi-scale modelling of the structure and mobility of small defect clusters in iron

William J Weber, Fei Gao, Ram Devanathan, Yanwen Zhang, Weilin Jiang, Multiscale Modeling and Experimental Validation of Radiation Effects in Silicon Carbide

Dilpuneet Aidhy, Tapan Desai, Taku Watanabe, Paul Millett, James Tulenko, Dieter Wolf, Simon Phillpot, Radiation Damage in Nanocrystalline UO₂

Syo Matsumura, Tomokazu Yamamoto, Taturou Takahashi, Aurore Guglielmetti, Alain Chartier, Kazuhiro Yasuda, Kennichi Shiyama, Kazufumi Yasunaga, Constantin Meis, Molecular dynamical study of Frenkel pairs in cerium dioxide

Wednesday Afternoon (2) -- Joint session with symposium 9

David Rodney, Thomas Nogaret, Marc Fivel, On the role of helical turns in the formation of clear bands in irradiated materials (S-9)

Tomohito Tsuru, Masatake Yamaguchi, Yoshiyuki Kaji, Clustering process and precipitation hardening in Fe-Cu alloys: First-principle and empirical model evaluations (S-6)

Yury Osetskiy, Atomic-scale modeling of dislocation-obstacle interactions in irradiated metals (S-6)

Yury Osetskiy, Dynamics of dislocation-localized obstacle interaction: what can we learn from atomic level modeling (S-9)

Emmanuel Clouet, Sébastien Garruchet, Hoang Nguyen, Michel Perez, Charlotte Becquart, Dislocation interaction with C in alpha-Fe: a comparison between atomic simulations and elasticity theory (S-9)

Stanislav Golubov, Study of Cavity Evolution in Iron under Neutron and Alpha-particle Irradiations (S-6)

Aleksandar Donev, Vasily Bulatov, First-passage Monte Carlo for materials under irradiation (S-6)

Thursday Morning

D Schwen, M. Huang, R. S. Averback, P. Bellon, An atomistic study of fission gas bubble re-resolution in UO₂.

Fei Gao, Ab initio Calculations of Defects, Defect Clusters and Defect Creation in SiC and GaN

Nicolas Castin, Lorenzo Malerba, **Giovanni Bonny**, Modelling radiation-induced phase changes in ternary Fe-Cu-Ni alloys using a Monte-Carlo Artificial Intelligence approach

Herbert Urbassek, **Luis Sandoval**, Influence of electronic stopping on sputtering induced by cluster impact on metallic targets

Dmitry Terentyev, Masood Hafez Haghighat, Robin Schäublin, Lorenzo Malerba, Interaction of dislocations with Cr-rich precipitates: a molecular dynamics study

Chaitanya Deo, Blas Uberuaga, Oxygen interstitial migration in hyperstoichiometric uranium dioxide studied by kinetic Monte Carlo simulations

Poster Presentations

Wednesday Afternoon

1. **Maria Okuniewski**, **Chaitanya Deo**, **James Stubbins**, Irradiation of helium implanted iron studied by multiscale modeling and experiments

2. **Giovanni Bonny**, Roberto Pasianot, Lorenzo Malerba, FeCuNi many-body potential consistent with thermodynamics
3. **Kazunori Morishita**, Yoshiyuki Watanabe , Akira Kohyama , Howard Heinisch , Fei Gao KMC simulations for formation kinetics of vacancy clusters in beta-SiC during irradiation
4. **Yoshiyuki Watanabe**, Kazunori Morishita, Akira Kohyama, Howard Heinisch, Fei Gao, Richard Kurtz, MD simulations for defect properties in β -SiC under irradiation
5. **Lianping Zhang**, Mengfu Wei, Lunqiang Wu, Lu Chunhai, The calculating analysis of the relationship between specialities of gamma spectrum and source condition
6. **Dmitry Terentyev**, Lorenzo Malerba, Characterization of dislocation loops, voids and Cr precipitates as competing sources of hardening in irradiated Fe-9Cr alloys
7. **Guillaume Lucas**, Robin Schäublin, Influence of helium on the clustering of self-interstitials in irradiated bcc iron
8. Maria Okuniewski, Chaitanya Deom, **James Stubbins**, Irradiation of helium implanted iron studied by multiscale modeling and experiments
9. **Zhiming Chen**, Zhiming Chen, Matous Mrovec, Daniel Weygand, Peter Gumbsch, Atomistic modeling of the interaction between dislocations and point defects in body-centered cubic iron
10. **Kenichi Nakashima**, Naoki Soneda, Akiyoshi Nomoto, Kinetic Monte-Carlo simulation of Irradiation Damage Accumulation in Strain Field of Dislocation
11. **Tomoaki Suzudo**, Mitsuhiro Itakura, Hideo Kaburaki, A Modeling Study of Grain Sub-division Observed at High Burnup Nuclear Fuel
12. **Pär Olsson**, Christophe Domain, Modelling of isochronal annealing in bcc metals