

Modeling of the behaviour of materials under irradiation

November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)



Detailed programme

NOMATEN Winter School 2021: programme

Tuesday, November 16, 2021

- 8:45 • Registration
- 9:00 • Welcome words, **Christophe GALLÉ** (CEA Saclay, France)
- 9:05 • General introduction of CEA, **Gilles MOUTIERS** (CEA Saclay, France)
- 9:20 • NOMATEN and the framework of the winter school, **Jacek JAGIELSKI** (NOMATEN-NCBJ, Poland)
- 9:30 • Introduction to the winter school: objectives and scientific contents / expectations,
- 9:45 **Mikko ALAVA** (NOMATEN-NCBJ, Poland), **Jean-Luc BÉCHADE** (CEA Saclay, France)
- 10:15 • Round table
Coffee break

SESSION 1: Lectures on basic notions on materials and irradiation, Part 1, Nov. 16TH, (A.M.)**Chairman: Lukasz KURPASKA, NOMATEN**

- 10:30 • Primary damage, point defects formation, migration and properties, cascades, **Jean-Paul CROCOMBETTE** (CEA Saclay, France)
- 11:45 • Thermodynamics, diffusion and phase stability under irradiation, **Maylise NASTAR**, (CEA Saclay, France)
- 13:00 Lunch Break

SESSION 2: Lectures on basic notions on materials and irradiation, Part 1, Nov. 16TH, (P.M.)**Chairman: Jean-Paul CROCOMBETTE, CEA**

- 13:45 • Plasticity at atomic scale, dislocations motion, irradiation defects interactions, **Emmanuel CLOUET**, (CEA Saclay, France)
- 15:00 • Nanoindentation and irradiated materials: technique, applications, results **Lukasz KURPASKA** (NOMATEN-NCBJ, Poland)
- 16:15 • Coffee break
- 16:30 • SAFIR BRUTE project - Barsebäck RPV material used for true evaluation of embrittlement, **Pentti ARFFMAN** (VTT, Finland)
- 17:45 Questions relative to organization
- 18:00 End of day 1

Detailed programme (continued)

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Wednesday, November 17, 2021

SESSION 3: Communications, Part 1, Nov. 17TH, (A.M.)

Chairman: Maria OKSA, VTT

9:00	• Welcome
9:05	• Frenkel pair accumulation in the molecular dynamics framework to study irradiation effects (in Fe, MgAl ₂ O ₄ , UO ₂ ...), Alain CHARTIER (CEA Saclay, France)
9:45	• Modelling irradiated materials: from Molecular Dynamics to Nanoindentation, Javier DOMINGUEZ (NOMATEN-NCBJ, Poland)
10:25	Coffee Break
10:40	• Interatomic potentials optimisation or crystalline defects determination using Machine Learning technics, Cosmin MARINICA (CEA Saclay, France)
11:20	• Materials Informatics of High Entropy Alloys, Stefanos PAPANIKOLAOU (NOMATEN-NCBJ, Poland)
12:00	Lunch Break

SESSION 4: Communications, Part 1, Nov. 17TH, (P.M.)

Chairman: Christophe GALLÉ, CEA

12:45	• Application of Calphad method (Zr base alloys, carbides, ...), Caroline TOFFOLON , (CEA Saclay, France)
13:25	• Solutes effects on the microstructural evolution of nickel base alloys as model alloy of austenitic steels, Marie LOYER-PROST (CEA Saclay, France)
14:05	• Nanoindentation of ion-irradiated materials and thin films, Lukasz KURPASKA (NOMATEN-NCBJ, Poland)
14:45	Coffee Break
15:00	• Corrosion modelling: Ekinox models, Laure MARTINELLI (CEA Saclay, France)
15:40	• Modelling of weld microstructure effect on brittle fracture initiation, Noora HYTÖNEN (VTT, Finland)
16:20	• Replacement chemicals for hydrazine in PWR secondary side cycles, Konsta SIPILÄ (VTT, Finland)
17:00	• Poster session 1
18:00	Free time
19:30	Welcome diner

Detailed programme (continued)

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Thursday, November 18, 2021

SESSION 5: Communications, Part 2, Nov. 18TH, (A.M.)**Chairman: Jean-Luc BÉCHADE, CEA**

9:00	• Welcome
9:05	• Dislocation interactions with irradiation defect-loops in metals, Laurent DUPUY (CEA Saclay, France)
9:45	• Multiscale modelling of plasticity with discrete dislocation dynamics, Mikko ALAVA (NOMATEN-NCBJ, Poland)
10:25	Coffee Break
10:40	• Impact of radiation damage on functional properties of alumina coatings deposited via PLD technique, Agata ZABOROWSKA (NOMATEN-NCBJ, Poland)
11:20	• Polycrystalline modeling of the behavior of neutron-irradiated recrystallized zirconium alloys during strain path change tests, Fabien ONIMUS (CEA Saclay, France)
12:00	Lunch Break

SESSION 6: Communications, Part 2, Nov. 18TH, (P.M.)**Chairman: M. ALAVA, NOMATEN**

12:45	• Utilizing micromechanical modeling as a part of the ICME workflow for irradiated materials, Matti LINDROOS (VTT, Finland)
13:25	• Interfaces, intergranular fracture prediction using multi-scale simulations, Laurent VAN BRUTZEL (CEA Saclay, France)
14:05	• Modelling of inhomogeneous fracture toughness behavior of irradiated reactor pressure vessel steels, Sebastian LINDQVIST (VTT, Finland)
14:45	Coffee Break
15:00	• Fracture behavior of austenitic stainless steels used for Pressurized Water Reactors (PWR) internals structures, Jérémy HURE (CEA Saclay, France)
15:40	• Study and modelling of tritium trapping in fusion relevant materials, Etienne HODILLE (CEA Cadarache, France)
16:20	• Unconventional application of microscopic techniques in analysis of irradiated materials, Iwona JÓŹWIK (NOMATEN-NCBJ, Poland)
17:00	• Poster session 2
18:00	End of the day

Detailed programme (continued)

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Friday, November 19, 2021

LECI hot laboratory, SCBM hot laboratories and JANNuS ion irradiation platform visits*, Nov. 19th, (a.m.), (*): limited participation / Organization to be confirmed

7:00	• Meeting at the main intrance of Luxembourg Garden in Paris and departure (by bus) to the East gate of CEA Saclay
8:30	• welcome and entrance procedure/formalities
9:30	• Visit of the LECI hot laboratory (DES/ISAS/DMN)
10:30	• Visit of SCBM hot laboratories (DRF/Joliot Institute)
11:30	• Visit of the JANNus Ion irradiation platform (DES/ISAS/DMN)
12:30	• Conclusion
12:45	Lunch (take-out boxes)
13:30	• End of the Winter School