European Funds

Republic of Poland

FNP Foundation for Polish Science

European Union

WINTER SCHOOL 2021

NOMATEN

Modeling of the behaviour of materials under irradiation

PARIS, Société Géologique de France
77 Rue Claude Bernard
NOVEMBER 16-19 2021

NCBJ

cea

VTT

NOMATEN

Centre of Excellence in Multifunctional Materials for Industrial and Medical Applications

WINTER SCHOOL PARIS 2021

SCOPE AND OBJECTIVE

The European NOMATEN project, launched at the end of 2019, aims to support the structuring and scientific influence of the NOMATEN Center of Excellence (CoE) dedicated to multifunctional materials for industrial and medical applications, created in Poland at the end of 2018.

In order to support the training of new generations of young Polish researchers (education programme) and to boost the growth of the NOMATEN CoE and its capacity to implement and manage research programmes, the first Winter School has been proposed. Organized by CEA, the first edition of the school is related to material sciences and takes place in Paris. It's agenda focuses on modeling and simulation of the behaviour of materials under irradiation - also confronted with experimental approaches.

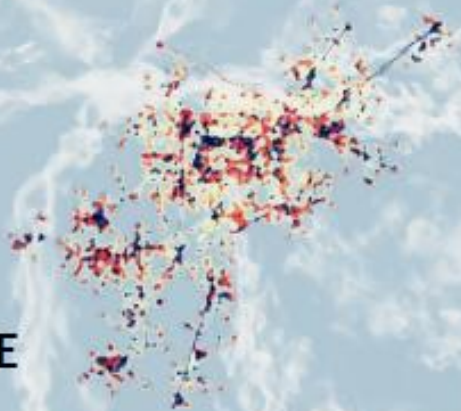
NOMATEN Winter School is designed for PhD, post-doctoral students and researchers with a priority for NOMATEN and NCBJ, VTT, CEA as well. Lasting four days, the school includes two sessions (1st day) dedicated to reminders and/or upgrades in the form of courses given by experts from CEA and VTT but also from NOMATEN CoE. Another two sessions (2nd & 3rd days) are dedicated to scientific communications from CEA, VTT and NOMATEN/NCBJ researchers. Additionally, two poster sessions will take place as well as the last day will be devoted to visits at selected CEA Saclay facilities.

SCIENTIFIC COMMITTEE

Jean-Luc Béchade, Christophe Gallé, Frédéric Dollé, Gilles Moutiers

Mikko Alava, Paweł Sobkowicz, Jacek Jagielski, Jacek Gajewski, Marcin Brykała

Maria Oksa



ORGANIZING COMMITTEE

Christophe Gallé, Christine Prouilhac, Jean-Luc Béchade, Frédéric Dollé, Gilles Moutiers

Modeling of the behaviour of materials under irradiation

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

NOMATEN Winter School 2021
Welcome Address

As members of the scientific committee of the NOMATEM winter school and on behalf of the organizing committee, we sincerely welcome you all to this school in Paris. This is the very first edition of this type of event in the frame of the European NOMATEN project and the associated Center of Excellence (CoE).

The NOMATEN Centre of Excellence (CoE) is a novel created (2020) polish research organization in which international world-class research teams will design, develop and assess innovative multifunctional structures: Novel high-temperature, corrosion and radiation resistant materials for industrial applications on one side, and novel radiopharmaceuticals for medical applications on the other side. Hosted by the National Centre for Nuclear Research (NCBJ, Swierck, Poland), the CoE involve by design a strong scientific partnership with the French Alternative Energies and Atomic Energy Commission (CEA, France) and the Technical Research Centre of Finland (VTT, Finland) with joint financial support from the Foundation for Polish Science (FNP) and the European Commission (the NOMATEN project).

As all of you are aware, this first school is related to the material sciences topic of NOMATEN, and the subject chosen for the first edition of such a joint event is “Modeling of the behavior of materials under irradiation”. This theme is not only essential in the objectives and the mission attributed to NOMATEM; It will also be a unique opportunity for all our junior scientists - doctoral and post-doctoral students - to meet and discuss together first, but more important, learn about basic notions in sciences of materials – especially under irradiation – coupled to the latest scientific developments carried out in our laboratories (CEA, VTT and of course NCBJ). Finally, a visit of three major facilities on the CEA Saclay site, two related to material sciences (the LECI hot laboratories, the JANNUS platform facility) and one related to radiopharmaceutical sciences (the SCBM laboratories) has been organized and will remain unforgettable for those who will attend it.

It is therefore our great honor and pleasure to have you here first in Paris, in the French Geological Society facilities, a few kilometers north from the CEA Paris-Saclay center, which we recall, is now an integral part of the new Paris-Saclay University, already ranked 13th worldwide and 1st in continental Europe. This world-class research-intensive university not only brings together ten constituent faculties and institutes, four Grandes Écoles, the Institut des Hautes Etudes Scientifiques, two associate institutions, but also shared laboratories with six national research organizations, including the CEA. With 48,000 students, 8,100 lecturers and 8,500 administrative and technical staff members, Université Paris-Saclay offers a comprehensive and varied range of undergraduate to doctorate level programmes and engineering degrees, renowned for their quality thanks to the reputation and commitment of the University’s academic staff.

This first edition of the NOMATEM School program is deliberately not organized digitally but physically in Paris – thanks to a slow down of the COVID-19 crisis – however with a reduced number of participants, mainly to fulfil restrictive criteria linked to the pandemia. Nevertheless, we will have the pleasure of welcoming about 60 people from Poland, Finland and France. Oral and poster contributions are all given in the booklet attached with the program, and with a summary detailing the content of each contribution.

As we are initiating the first school within the European NOMATEN project, we are quite confident that we will have great time during this event in 2021. We hope all of you will enjoy fruitful discussions during this winter school, and wish you an enjoyable and safe stay in Paris.

On behalf of the local organizing committee
Christophe Gallé, Jean-Luc Béchade, and Frédéric Dollé

Modeling of the behaviour of materials under irradiation

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

Modeling of the behaviour of materials under irradiation

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

The French Geological Society is welcoming us in Paris

The Geological Society of France (SGF), a learned society founded on March 17, 1830, recognized as being of public utility, aims to contribute to the development of Earth and Planetary Sciences, both in itself and in its relations with industry, agriculture. , environment and education. SGF also offers nice facilities for hosting small-sized schools and is located in the center of Paris, close to the Luxembourg gardens.

Société Géologique de France (SGF), 77 Rue Claude Bernard, 75005 Paris

Modeling of the behaviour of materials under irradiation

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

About lectures, communications and poster sessions ...

Please note that all lectures and communications will be given in the conference room (salle Van Straelen).

Please note that poster sessions will be organized in the library lecturer room (salle de lecture de la bibliothèque), just in front of the conference room.

About coffee breaks and lunches ...

Please note that all caffee breaks will also be served in the back of the conference room (salle Van Straelen).

Please note that all lunches will be served in the library lecturer room (salle de lecture de la bibliothèque), just in front of the conference room, at the exception of the last day, where lunch boxes will be provided at the CEA Paris-Saclay before living the site.

About the welcome diner ...

For those of you that reserved for this diner, please remind that the location is the POLIDOR restaurant, 41 Rue Monsieur le Prince, 75006 Paris (https://www.polidor.com), which is located walking distance from the French Geological Society building.

About sanitary issue (Covid-19)

Restrictions are still in force in metropolitan France. Thus, while you are in France you will need to present a “health pass (Covid-19)” for access to certain events and places, currently all cafés, bars and restaurants, whether indoors or on the terrace, as well as in some shopping malls. It is also mandatory on board airplanes, trains and long-distance buses, as well as for access to all events or leisure and cultural places receiving more than 50 people (theaters, cinemas, museums, concert halls, festivals …).. Nationals of European Union countries have a digital “Covid certificate” (QR code) accepted in France. More informations: https://www.gouvernement.fr/en/coronavirus-covid-19

Modeling of the behaviour of materials under irradiation

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

Detailled 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, **Christophe GALLÉ, Frédéric DOLLÉ** (CEA Saclay, France)
9:20	•	NOMATEN Teaming project and the framework of the Winter School, **Jacek JAGIELSKI** (NOMATEN-NCBJ, Poland)
9:30	•	Introduction to the winter school: objectives and scientific contents / expectations, **Jean-Luc BÉCHADE** (CEA Saclay, France), **Mikko ALAVA** (NOMATEN-NCBJ, Poland)
9:45	•	Round table
10:15		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 (Library room)

SESSION 2: Lectures on basic notions on materials and irradiation, Part 2, 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

Modeling of the behaviour of materials under irradiation

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

Detailled programme (continued)

NOMATEN Winter School 2021: programme

Wednesday, November 17, 2021

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

Chairman: Maria OKSA, VTT

8:45	• Welcome
9:05	• Frenkel pair accumulation in the molecular dynamics framework to study irradiation effects (in Fe, $MgAl_2O_4$, UO_2…), **Alain CHARTIER** (CEA Saclay, France)
9:45	• Modelling irradiated materials: from molecular dynamics to nanoidentation, **Javier DOMINGUEZ** (NOMATEN-NCBJ, Poland)
10:25	Coffee Break
10:40	• Machine learning for atomistic materials science, **Cosmin MARINICA** (CEA Saclay, France)
11:20	• Materials informatics of high entropy alloys, **Stefanos PAPANIKOLAOU** (NOMATEN-NCBJ, Poland)
12 :00	• Quantitative microscopy for multiscale modelling, **Wade KARLSEN** (VTT, Finland)
12:40	Lunch Break (Library room)

SESSION 4: Communications, Part 2, Nov. 17TH (P.M.)

Chairman: Christophe GALLÉ, CEA

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	• Development of thermodynamic tools for Zr base alloys using the Calphad method, **Caroline TOFFOLON** (CEA Saclay, France)
15:40	• Corrosion modelling: Estimation KINetics OXidation code, **Laure MARTINELLI** (CEA Saclay, France)
16:20	Break
16:45	• **Poster session 1** (Library room) • Evaluation of alternative oxides as a strengthening particles for ODS Reduced Activation Ferritic steels, **Małgorzata FRELEK-KOZAK *et al.*** (NOMATEN-NCBJ, Poland) • The influence of manufacturing parameters on microstructure and mechanical properties of CoCrFeNi high entropy alloys produced via Mechanical Alloying and Spark Plasma Sintering, **Artur OLEJARZ *et al.*** (NOMATEN-NCBJ, Poland) • Experimental and computational study of intrinsic mechanical properties of pristine and irradiated Fe, **Katarzyna MULEWSKA *et al.*** (NOMATEN-NCBJ, Poland)

Modeling of the behaviour of materials under irradiation

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

- Understanding oxidation of zirconium and its alloys in air and water vapour operating conditions, **Kinga SUCHORAB *et al.*** (NOMATEN-NCBJ, Poland)
- Transmission Electron Microscopy as a tool for studying defects of irradiated materials, **Witold CHROMIŃSKI** (NOMATEN-NCBJ, Poland)
- NOMATEN's XRAYLAB – The newly-created X-Ray diffraction laboratory, **Maciej ZIELIŃSKI** (NOMATEN-NCBJ, Poland)
- Annealing-induced strengthening in the NiCoCr alloy: The role of segregation, **Axel POISVERT *et al.*** (NOMATEN-NCBJ, Poland)
- Molecular dynamics simulation of interface structure and shape of Nb precipitate in Zr matrix, **Zhengxuan FAN *et al.*** (CEA Saclay, France)
- Thermodynamic modeling of Ti-O from ab initio calculations, **Martin-Stéphane TALLA NOUTACK *et al.*** (CEA Saclay, France)
- Replacement chemicals for hydrazine in PWR secondary side cycles, **Konsta SIPILÄ** (VTT, Finland)

17:45	Free time
19:30	Welcome dinner (POLIDOR restaurant, 41 Rue Monsieur le Prince, 75006 Paris)

Modeling of the behaviour of materials under irradiation

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

Detailled programme (continued)

NOMATEN Winter School 2021: programme

Thursday, November 18, 2021

SESSION 5: Communications, Part 3, Nov. 18TH (A.M.)

Chairman: Jean-Luc BÉCHADE, CEA

8:45	•	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	•	Utilizing micromechanical modeling as a part of the ICME workflow for irradiated materials, **Matti LINDROOS** (VTT, Finland)
12:40		Lunch Break (Library room)

SESSION 6: Communications, Part 4, Nov. 18TH (P.M.)

Chairman: M. ALAVA, NOMATEN

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		Break
17:10	•	**Poster session 2** (Library room)
	•	Structure-based optimization of crystal plasticity parameters in metal alloys, **Karol FRYDRYCH *et al.*** (NOMATEN-NCBJ, Poland)
	•	Shear banding instability in high entropy multi-component metallic glasses: The role of composition and order, **Kamran KARIMI *et al.*** (NOMATEN-NCBJ)

Modeling of the behaviour of materials under irradiation

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

	• Features of solid solution hardening in face-centered cubic random high entropy alloys: MD simulation, **Amin ESFANDIARPOUR BOROUJENI *et al.*** (NOMATEN-NCBJ, Poland) • Configurational entropy in high entropy metallic glasses, **Rene A. ALVAREZ DONADO *et al.*** (NOMATEN-NCBJ) • Discrete dislocation dynamics simulations with free surfaces: Applicaton to mechanical testing of micropillars, **Fabrizio ROVARIS *et al.*** (NOMATEN-NCBJ, Poland) • Structural, mechanical and electrical properties of ion-irradiated polymers used as cable insulation, **Anna KOSIŃSKA *et al.*** (NOMATEN-NCBJ, Poland) • Synthesis of high-entropy alloy coatings obtained by magnetron sputtering, **Magdalena WILCZPOLSKA *et al.*** (NOMATEN-BCBJ, Poland) • Challenges concerning industry partnerships and communication towards companies, science and public sector, **Maciej DROZD *et al.*** (NOMATEN-NCBJ, Poland) • Crystal plasticity law calibration of non-irradiated and proton irradiated 304L austenitic stainless steel, **Rachma AZIHARI *et al.*** (CEA Saclay, France) • Study of Ni based alloys obtained by Additive Manufacturing, **Martin MADELAIN *et al.*** (CEA Saclay, France)
18:00	End of the day

Modeling of the behaviour of materials under irradiation

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

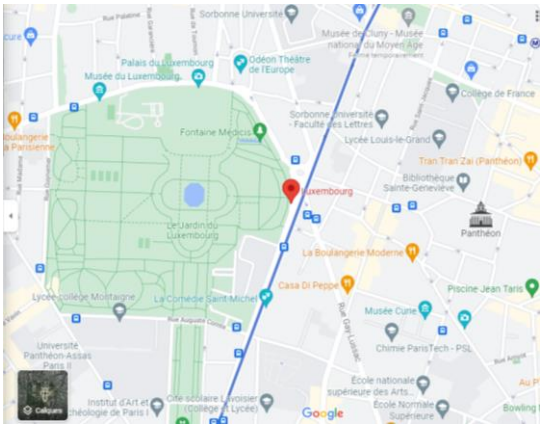
Detailled programme (continued)

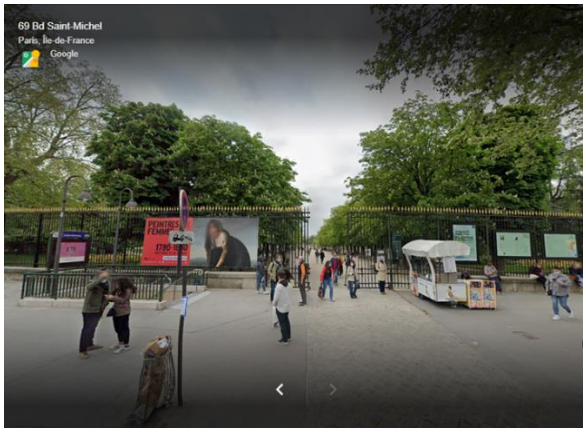
NOMATEN Winter School 2021: programme

Friday, November 19, 2021

LECI hot laboratory, SCBM hot laboratories and JANNuS ion irradiation platform visits, nov. 19TH (A.M.).

6:45	•	Meeting at the main entrance of Luxembourg Gardens in Paris and departure (by bus) to the North gate of CEA Saclay
8:15	•	welcome and entrance formalities ***
9:00	•	Visit of the LECI hot laboratory (DES/ISAS/DMN, B625)
10:15	•	Visit of SCBM hot laboratories and coffee break (DRF/Joliot Institute, B547)
11:45	•	Visit of the JANNuS Ion irradiation platform (DES/ISAS/DMN, B126)
12:45	•	Conclusion (farewell message)
13:00		Lunch (take-out boxes provided in the JANNuS Hall)
13:30	•	End of the Winter School and departure to Paris by bus





Meeting point at the main entrance of Luxembourg Gardens (St Michel Boulevard, Paris 6e)

****** reminder, entry at the CEA Paris-Saclay request the presentation (compulsory) of a valid identity document (IC or passport).***

Modeling of the behaviour of materials under irradiation

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

Abstracts of the Lecture
(Tuesday, November 16, Parts1 & 2)

Modeling of the behaviour of materials under irradiation

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

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Modelling of the promary damage and the properties of point defects

Jean-Paul CROCOMBETTE

Université Paris-Saclay, CEA, Service de Recherche en Métallurgie Physique, 91191 Gif-sur-Yvette cedex, France

Abstract
In this lecture, we want in a first part to address the various aspects of the modelling of the primary damage of irradiation and, in a brief second part to describe how one can calculate the basic formation and migration properties of the defects created by irradiation. The methodologies of each modelling step will be briefly recalled, the tools and codes used in CEA will be presented and the results will illustrated with examples from CEA's studies.

The simulation of primary damage starts with the determination of Primary Knocked-on Atom (PKA) spectrum for a given neutron flux. We use the DART code (Luneville et al. 2006), which also enables to study which ion beam could be contemplated to reproduce approximately a given neutron flux. Once the PKA spectrum (or ion energy) is determined, the primary damage modelling aims to describe the collision cascades created by the PKAs, and to obtain the amount and nature of created defects. In the case of ion irradiation, one is also interested in the spatial distribution of damage and ion implantation. There are two complementary simulation framework:

- The Binary Collision Approximation (BCA) which is specifically devoted to the modelling of irradiation damage. Some details will be given about these simulations. In particular, we will discuss the differences between and respective advantages of the so-called Full cascade and Quick-Calculations of damage in connection with NRT standard of damage creation. For ion irradiations, this modelling relies heavily on the famous SRIM code. We shall present the IRADINA code (Crocombette et al. 2019) which has been developed by the university of Jena and adapted by CEA to a nuclear context. We believe Iradina can be a nice alternative to the ageing SRIM.
- The Molecular Dynamics with empirical potential is the complementary tool. MD allows for a much more detailed description of the collision cascades. MD simulation provide a detailed description of the structure of cascade created defects as well as a much more precise evaluation of the number of these defects. The well-known overestimation of the number of defects by BCA simulations and NRT standard has recently led to a proposition of new standard, the so-called arc-dpa (Nordlund et al. 2018), which we shall present and briefly discuss.

Both simulation methodologies rely on the distinction between electronic and ballistic loses for the fast moving atoms. The electronic stopping power is usually tabulated. However in the recent years, Time Dependent Density Functional Theory (TD-DFT) has been used to calculate it ab initio. We shall mention the MolGW code (Maliyov et al. 2018), which implements TD-DFT to calculate electronic stopping power in an atomic basis.
The properties of defects we are interested in in the context of irradiation damage are their structure, and their formation and migration energies. DFT is the method of choice to study these properties. It usually proceeds through super-cell calculations. We shall introduce the ANETO code (Varvenne et al. 2013), which improves the convergence of the calculations with respect the supercell size considering the elastic dipole of the defects. With the same tool, noticeable stress effects on the migration barriers can be obtained which can be important for later microstructural evolution. DFT calculations are usually performed at 0K. Finite temperature can naturally affect the properties of defects. This will be illustrated with the PAFI code (Swinburne et al. 2018) for the calculation of finite temperature energy barriers.

We shall end-up with an introduction to a method that bridges the atomic-description of defects and the modelling of microstructure evolution while bypassing the detailed description of primary damage. Indeed the accumulation of Frenkel pairs within empirical potential MD has proven a valuable methodology to evaluate the possible microstructure evolution of a crystal under irradiation. This methodology will be presented in details I

latter talk, but we shall introduce it with the case of the variation, with temperature and composition, of the amorphization dose of oxides (Chartier et al. 2009).

References

[A. Chartier, G. Catillon et J. P. Crocombette2009] A. Chartier, G. Catillon et J. P. Crocombette, *Key Role of the Cation Interstitial Structure in the Radiation Resistance of Pyrochlores,* Physical Review Letters **102**: 155503 (2009).

[J.-P. Crocombette et C. Van Wambeke2019] J.-P. Crocombette et C. Van Wambeke, *Quick calculation of damage for ion irradiation: implementation in Iradina and comparisons to SRIM,* EPJ Nuclear Sci. Technol. **5,** (2019).

[L. Luneville, D. Simeone et C. Jouanne2006] L. Luneville, D. Simeone et C. Jouanne, *Calculation of radiation damage induced by neutrons in compound materials,* Journal of Nuclear Materials **353**: 89-100 (2006).

[I. Maliyov, J.-P. Crocombette et F. Bruneval2018] I. Maliyov, J.-P. Crocombette et F. Bruneval, *Electronic stopping power from time-dependent density-functional theory in Gaussian basis,* The European Physical Journal B **91**: 172 (2018).

[K. Nordlund, S. J. Zinkle, A. E. Sand, F. Granberg, R. S. Averback, R. E. Stoller, T. Suzudo, L. Malerba, F. Banhart, W. J. Weber, F. Willaime, S. L. Dudarev et D. Simeone2018] K. Nordlund, S. J. Zinkle, A. E. Sand, F. Granberg, R. S. Averback, R. E. Stoller, T. Suzudo, L. Malerba, F. Banhart, W. J. Weber, F. Willaime, S. L. Dudarev et D. Simeone, *Primary radiation damage: A review of current understanding and models,* Journal of Nuclear Materials **512**: 450-479 (2018).

[T. D. Swinburne et M. C. Marinica2018] T. D. Swinburne et M. C. Marinica, *Unsupervised Calculation of Free Energy Barriers in Large Crystalline Systems,* Phys Rev Lett **120**: 135503 (2018).

[C. Varvenne, F. Bruneval, M. C. Marinica et E. Clouet2013] C. Varvenne, F. Bruneval, M. C. Marinica et E. Clouet, *Point defect modeling in materials: Coupling ab initio and elasticity approaches,* Physical Review B **88**: 134102 (2013).

Modeling of the behaviour of materials under irradiation

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

Thermodynamics, diffusion and phase stability under irradiation

Maylise NASTAR

Université Paris-Saclay, CEA, Service de Recherche en Métallurgie Physique, 91191 Gif-sur-Yvette cedex, France

Abstract

To illustrate the modeling of phase stability under irradiation, we rely on a recent theoretical and experimental investigation of the dilute cubic-centered phase Fe(Ni) alloy [1]. Atom probe tomography and transmission electron microscopy investigations report an effect of the Fe-ion irradiation on the redistribution of Ni close to voids and dislocation loops. At higher radiation dose, one observes large precipitates of the austenite γ phase, that is not predicted by the phase diagram. This phase transformation is the consequence of the long time evolution of the numerous Frenkel pairs of point defects (vacancy and Self-Interstitial Atom (SIA)) left after the primary radiation damage. Through this example, we will give an overview of the multiscale approaches followed nowadays to model the evolution of metallic alloy microstructures under irradiation. Many lengths and time scales are involved, starting from the creation, migration, and elimination reactions of point defects at the atomic scale, to their long-range diffusion leading to the formation of point defect clusters such as voids and dislocation loops, mixed solute-point defect nano-clusters and the precipitation of stable or metastable secondary phases. In addition, the sustained fluxes of point defects towards the extended defects of the microstructure may also yield to local solute redistributions at these point defect sinks. This is the so-called radiation induced segregation [2]. The impact of the microstructure evolution on the macroscopic material properties is multiple, such as dimensional changes of the component, a lower or higher resistance to corrosion and the modification of the mechanical properties. Depending on their time and spatial scales, the kinetic events described above require different modeling techniques. The formation of Frenkel pairs within a displacement cascade occurs at the time scale of a few picoseconds. Whereas, the vacancy in Fe at 400 °C, takes 1 microseconde to diffuse over a few nanometers through a series of first nearest neighbor atom-vacancy exchanges. Kinetics events controlled by the diffusion of point defects requires simulation methods at the time scale of the atom-point defect exchange. The latter is a thermally activated process associated with an activation barrier and an attempt frequency, which one determines from the transition state theory. At this scale, the vibrational frequencies of the atoms are not explicitly treated. They are accounted for as an entropic contribution to the exchange activation barrier and the formation enthalpy of the point defect. Thermally activated events lead the system towards the equilibrium state, while the a-thermal events such as the creation of Frenkel pairs, the forced atomic relocations, the recombination reactions between point defects and the elimination of point defects at sinks drive the system towards a non equilibrium steady state. The radiation-induced microsctructure is a non equilibrium microstructure resulting from the competition between thermal and athermal kinetic events. On-lattice simulation techniques such as the atomic kinetic Monte Carlo method, tackle this competition at the atomic scale [3]. This method covers timescale fixed by the atom-point defect exchange frequencies and volumes containing around one million of atoms (corresponding to simulation box sides of around 20 nm). In such volumes, the simulation of a reasonable concentration of point defects implies that only one or two point defects operate in the simulation box. To simulate the evolution of a point defect clusters distribution, we may rely on object kinetic Monte Carlo methods or mean field rate theories [4]. These are mesoscopic techniques that do not require an on-lattice modeling of the point defect reactions, but the interactions between point defects and solutes is poorly described. In particular, kinetic phenomena such as the precipitation of a semi-coherent phase, the loss of coherency of precipitates, require an off-lattice modeling of the coupled solute-point defect kinetic events. The phenomenological thermodynamics of irreversible processes is a thermodynamic formulation of the kinetic events that can be extended to the modeling of driven phase transformations in irradiated systems. The corresponding thermodynamic and kinetic parameters, when derived from the atomic scale, include the effects of a-thermal events [1,5]. The latter are introduced as non-equilibrium constraints affecting the diffusion properties and the thermodynamic driving forces. By relying on the atomic scale characterization of the Fe-Ni system, we present the different steps of a multi-scale modeling scheme aiming at predicting the solute redistribution and point defect clustering resulting from radiation induced segregation and precipitation phenomena.

Modeling of the behaviour of materials under irradiation

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

1. Experimental investigation of the Fe-Ni system under irradiation
   We introduce the various mechanisms of solute redistribution that occurr in the ion irradiated ferritic Fe(Ni) alloy.
2. Thermodynamic driving forces of the alloy and lattice point defects under irradiation
   We briefly present the atomic Monte Carlo methods, statistical physics models and the CALPHAD approach, that are currently employed to model the thermodynamic properties of alloys and lattice point defects. Under irradiation, point defects are not at equilibrium. We show how to build a constrained thermodynamic formulation accounted for the effect of a non equilibrium concentration of point defects. The diffusion and precipitation driving forces become then a function of the point defect chemical potential, the atomic density of phases, and the alloy thermodynamics. On the Fe-Ni example, we illustrate the role of point defects from the calculation of the constrained phase diagram and the resulting driving forces.
3. Diffusion mechanisms and phenomenological transport coefficients under irradiation
   By relying on the thermodynamics of irreversible processes formulation, we explain why diffusion experiments are not sufficient to understand point defect solute flux couplings. The latter require the calculation of the full Onsager matrix of the phenomenological transport coefficients. We present a combined *ab initio*-KineCluE analysis of the flux couplings in Fe-Ni.
4. Modeling the synegertic kinetics of point defects, precipitates and point defect clusters
   We show how to derive kinetic laws for the evolution of the point defect concentration in interaction with the growth of semi-coherent precipitates and point defect clusters. We rely on the phenomenological transport coefficients, the constrained Gibbs free energies of phases, and the enthalpy of formation of point defects.
5. Radiation induced segregation as a nucleation catalyst of semi-coherent precipitation
   RIS in alloys results from the net flux of point defects, which is sustained by the production and elimination reaction of point defects at the extended defects. Solute atoms segregate because the net flux of point defects toward extended defects induces fluxes of the various atomic species. On the example of Fe-Ni, we will show how the radiation induced segregation of Ni triggers the precipitation of the γ phase.

References

[1] M. Nastar, L. Belkacemi, E. Meslin, M. Loyer-Prost, Thermodynamic model for lattice point defect-mediated semi-coherent precipitation in alloys, Communication Materials 2 (2021) 32.
[2] M. Nastar and F. Soisson, Radiation induced segregation, Comprehensive Nuclear Materials (2020).
[3] F .Soisson, E. Meslin, O. Tissot, Atomistic modeling of α'precipitation in Fe-Cr alloys under charged particles and neutron irradiations: Effects of ballistic mixing and sink densities Journal of Nuclear Materials 508 (2018) 583.
[4] D. Carpentier, T. Jourdan, P. Terrier, M. Athenes, Y. Le Bouar, Effect of sink strength dispersion on cluster size distributions simulated by cluster dynamics, J. of Nuclear Materials, 533 (2020), 152068.
[5] L. Huang, M. Nastar, T. Schuler, L. Messina, Multiscale modeling of the effects of temperature, radiation flux, and sink strength on point-defect and solute redistribution in dilute Fe-based alloys, Phys. Rev. M 5 (2021) 033605.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Crystal plasticity at the atomic scale

Emmanuel CLOUET

Université Paris-Saclay, CEA, Service de Recherche en Métallurgie Physique, 91191 Gif-sur-Yvette cedex, France

Abstract

Plasticity of crystal materials is mainly controlled by the motion of dislocations, i.e. line defects carrying shear increments. Although elasticity theory [1,2] allows rationalizing a large part of dislocation behavior, in particular their long-range interactions, some of their fundamental properties like their glide plane and their mobility highly depend on their core. This core region corresponds to the immediate vicinity of the defect where the perturbation of the crystal is too important to be described by elasticity. The modelling of this core region necessitates an atomic description, and atomistic simulations have thus become a valuable tool to study dislocation properties.

Such simulations can rely either on ab initio calculations or on empirical potentials, these two approaches offering different potentialities with a balance between the needed accuracy for the description of atomic bonding and the size of the system to model. In this lecture, we will review how both approaches can be used to model dislocations at the atomic scale and to build a multiscale approach of plasticity starting from an atomic description. The lecture will be illustrated by examples coming from studies in body-centred cubic (bcc) and hexagonal close-packed (hcp) transition metals, like Fe and Zr, which are the base of alloys largely used as structural materials in the nuclear industry.

Ab initio calculations based on the density functional theory (DFT), as they rely on an electronic description of the atomic bonding, appear as the most accurate and predictive simulation tools. As these calculations are still limited in the size of the system they can handle, typically at most a few hundred atoms, the ab initio modelling of dislocations need special attention. Specific methodologies have been therefore developed to study dislocation core properties with ab initio calculations [3,4]. Starting from the modelling of dislocations in the pure metal and the determination of the energy barriers opposing their glide, one can build mobility laws for these dislocations and predict the temperature- and orientation-dependence of the single-crystal yield stress in the thermally activated regime where plasticity is governed by the glide of screw dislocations through nucleation and propagation of kink-pairs [5]. Such ab initio calculations also allow studying the interaction of dislocations with solute atoms, to model then the impact of solute addition on dislocations mobility.

The use of empirical interatomic potentials instead of ab initio calculations allow handling much larger simulation cells. It becomes then possible to simulate the glide of long dislocations through molecular dynamics, thus without supposing a priori the mechanism controlling the dislocation motion. More complex situations involving several dislocations can also be accessed, to evidence the interaction and the possible reactions between dislocations or between dislocations and irradiation defects.

References

[1] Hirth J.P., Lothe J. Theory of dislocations, 2nd edn. (Wiley, New York, 1982).

[2] Bacon D.J., Barnett D.M., Scattergood R.O. Anisotropic continuum theory of lattice defects, Prog. Mater. Sci. **23**, 51–262 (1980).

[3] Rodney D., Ventelon L., Clouet E., Pizzagalli L., Willaime F. Ab initio modeling of dislocation core properties in metals and semiconductors. Acta Mater **124**, 633–659 (2017).

[4] Clouet E. Ab initio models of dislocations, in Handbook of materials modeling (Springer, 2018).

[5] Clouet E., Bienvenu B., Dezerald L., Rodney D. Screw dislocations in BCC transition metals: from ab initio modeling to yield criterion, C. R. Phys. **22**, S3 (2021).

Modeling of the behaviour of materials under irradiation

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

Nanoindentaion and irradiated materials: technique, applications

Łukasz KURPASKA

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland

Abstract

From the historical poin of view the nanoindentation method have been introduced in 1992. At the beginning this technique was devoted to measuring hardness and elastic modulus by instrumented indentation experiment procedure. Since its original development, the method has undergone numerous refinements and changes. These brought improvements to testing equipment and techniques as well as improve our understanding of the elastic–plastic contact point. I will review our current understanding of the method and provide an update of how we now implement it so to make the most accurate mechanical property measurements [1]. The limitations of the method, with special emphasis on thin layers (ion irradiation can also be treated as a multi-layer system) systems will be discussed.

In the second part of my talk I will focuse on indentation with spherical indenter. Although these experiments have long been used to measure the hardness and Young's modulus, the utility of this technique in analyzing the complete elastic–plastic response of materials under contact loading has only been realized in the past few years. This could be done due to recent advances in analysis protocols.

In this lecture I will review basic idea of the spherical experiment procedure and provide infromation in respect to extracting meaningful indentation stress–strain curves from the raw datasets. These indentation stress–strain curves have produced highly reliable estimates of the indentation modulus and the indentation yield strength in the sample [2]. These are the most basic parametrs which must be determined in order to properly assess impact of radiation defect on the mechanical properties and structural integrity of the components.

Final part on my talk will be related to nanoindentation measurement capabilities at elevated temperatures. These have developed considerably over the last ten years. Commercially available systems can now perform stable indentation testing at temperatures even up to 800 or 1000 °C (NCBJs system, up to 650 °C) with thermal drift levels similar to those present at room temperature [3]. I will discuss the thermal management and measurement techniques necessary to conduct valuable indentation at high temperature.

Special emphasis will be put on independent heating of both the indenter and the sample. Finally, problem of oxidation of the indenter and/or sample will be presented. A natural extension of testing in vacuum or Ar-like atmosphere in elevated temperature, is nanoindentation in situ in the scanning electron microscope. One of the solutions currnelty available in the market will be discussed too.

References

[1] W.C. Oliver et al., "Measurement of hardness and elastic modulus by instrumented indentation: Advances in understanding and refinements to methodology", Journal of Materials Research 19 (2004).

[2] S. Pathak et al., "Spherical nanoindentation stress–strain curves", Materials Science and Engineering R 91 (2015).

[3] J.M. Wheeler et al., "High temperature nanoindentation: The state of the art and future challenges", Current Opinion in Solid State and Materials Science 19 (2015) 354.

Modeling of the behaviour of materials under irradiation

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

SAFIR BRUTE Project – Barsebäck RPV material used for true of embrittlement evaluation

Pentti ARFFMAN

VTT Technical Research Centre of Finland, P.O. Box 1000, FI-02044 VTT, Finland

Abstract

BRUTE is a research project within the Finnish national nuclear research programme SAFIR. The project has been ongoing since 2018 and is planned to finish in the end of 2022. It works as an extension of the BREDA programme, aimed to utilize the decommissioned Barsebäck 2 (B2) nuclear power plant in evaluation of BWR safety. In addition to SAFIR, BRUTE has received funding from Swedish NKS programme.

The project BRUTE has two primary objectives. First, commissioning of new research facilities at VTT CNS have meant introduction of new equipment. The facilities and equipment require training, and new hot cells require new tools, applicators etc. Once the equipment and practises are familiar, validation tests must be performed for each test method. Quality control includes accreditation with annual external inspections. This process was a major part of BRUTE during the first half of the project. On the other hand, characterisation of material extracted from B2 enables comparison to the surveillance program results, providing thus a potential validation to the safety of similar BWRs. BRUTE aims to demonstrate the correlation between surveillance material and the true material extracted from the RPV. Secondary objectives include intensified Nordic collaboration by means of meetings, workshops. An international seminar in under consideration for 2023. Furthermore, a generational shift is ongoing in nuclear research. BRUTE acts as a means for the young generation to familiarize themselves with people and methods in the industry, learn from the experienced, and finally take the reins. This also includes academic development: a Master's thesis has been produced in the project, and a dissertation in under work. Scientific publications will be prepared from all valuable discoveries.[1]

The test program of BRUTE has focused on the weld metals in the pressure vessel. Mechanical and fracture mechanical test program includes tensile tests, impact tests and brittle fracture testing. Tensile tests are performed with flat miniature specimens, using laser illumination to produce a speckle pattern in the specimen. The measurements are able to closely trace material behaviour in the yield region, something that has not always been possible with older equipment. Impact testing is conducted with an instrumented hammer tip. In addition to the conventional impact energy, this provides detailed information of the dynamic fracture phenomenon. Different characteristic points in the load-displacement curve correlate with different events during impact. Fracture mechanical tests are performed utilising the master curve methodology, aimed at determining the brittle fracture transition temperature.[2] In addition to the regular master curve methodology, the individual tests are analysed more thoroughly to obtain further knowledge and for quality control. Furthermore, test series are screened for inhomogeneity and evaluated using corresponding methods, if needed. While the standard information obtained from mechanical and fracture mechanical tests may provide a good starting point for modelling of material behaviour, more information is required to improve the models. Instead of performing new tests, the material response signals may provide much of this information, if the analysis is improved.

Microstructural investigations within BRUTE include metallography, spectroscopy and various electron microscopy investigations, among others. The analysis of initiation sites, inclusions, grain sizes and types enhance the material knowledge from simple numbers to much more detailed evaluation. The merger of mechanical test results and fractographical investigations, along with statistical analysis of them provides superior material information for modelling.

Modeling of the behaviour of materials under irradiation

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

References

[1] N. Hytönen *et al.*, "Effect of weld microstructure on brittle fracture initiation in the thermally-aged boiling water reactor pressure vessel head weld metal," *International Journal of Minerals, Metallurgy and Materials*, vol. 28, no. 5, pp. 867–876, 2021, doi: 10.1007/s12613-020-2226-6.

[2] S. Lindqvist and T. Seppänen, "BREDA: Fracture toughness measurements with miniature C(T) specimens in reference condition," 2017.

Modeling of the behaviour of materials under irradiation

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

Abstracts of the communications
(Wednesday, November 17, Parts 1 & 2)

Modeling of the behaviour of materials under irradiation

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

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Frenkel pair accumulation in the molecular dynamics framework to study irradiation effects

Alain CHARTIER

Université Paris-Saclay, CEA, Service de la Corrosion et du Comportement des Matériaux dans leur Environnement, 91191 Gif-sur-Yvette cedex, France

Abstract

Molecular dynamics simulation of radiation damages in materials frequently refer to studies in which displacement cascades, threshold displacement energies and sometimes, thermal spikes are performed. Each of these techniques are meant to address the primary damage – i.e. single events – produced by electronic loss and/or ballistic interactions. Recent attempts have tried to explore the effect of the irradiation dose by accumulating these single events. However, this demarche is limited to low doses (0.1 dpa) since very cpu demanding. One may circumvent single events and access higher doses – in some specific cases – by shortcutting part of the story. Instead of repeating 'single event' one after the other to get the effect of dose, the final state can be used as a starting point.

Here, we show that as long as single events end up with point defects or very small clusters, it is convenient to accumulate point defects to reach doses up to 10 dpa or more [1]. Such a simulation procedure opens highways for understanding complicated mechanisms at work when materials are in severe irradiation environments. For example, one can (i) identify the specific defect responsible for amorphization in titanate pyrochlores [1], (ii) shed light on the wrinkling responsible for the anisotropic swelling in graphite [2], (iii) exhibit Frank loops as part of the monitoring mechanism for UO2 swelling [3], or (iv) evidence that C15 clusters are seeds for both ½ <111> and <100> loops [4].

References

[1] A. Chartier, G. Catillon, and J.-P. Crocombette, Phys. Rev. Lett. 102 (2009) 155503.

[2] A. Chartier, L. Van Brutzel, B. Pannier, and P. Baranek, Carbon 91 (2015) 395.

[3] A. Chartier, C. Onofri, L. Van Brutzel, C. Sabathier, O. Dorosh, and J. Jagielski, Appl. Phys. Lett. 109 (2016) 181902.

[4] A. Chartier, and M.C. Marinica, Acta Mater. 180 (2019) 141.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Modelling irradiated materials: from Molecular Dynamics to nanoindentation

Francisco Javier DOMÍGUEZ-GUTIÉRREZ[a,b,*], Stefanos PAPANIKOLAOU[a], Amin ESFANDIARPOUR[a], Pawel SOBKOWICZ[a], M. ALAVA[a,c]

[a]NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Otwock, Poland
[b]Institute for Advanced Computational Science, Stony Brook University, Stony Brook, NY 11749, USA
[c]Department of Applied Physics, Aalto University, P.O. Box 11000, 00076 Aalto, Espoo, Finland

Abstract

The development of novel technology in aerospace and energy industries requires the use of materials that can sustain extreme operating environments with high temperature and under irradiation. Molybdenum is selected as a candidate for its high melting point and good resistance to deformation under plasma irradiation. In this work, we perform Molecular Dynamics (MD) simulations to emulate neutron irradiation in crystalline Mo to investigate Frenkel pairs and crowdion formation at different primary knock-on atom energies by EAM and Gaussian Approximation potentials frameworks, obtained results are shown in Fig 1 and 2. Besides, we study the thermomechanical stability of molybdenum at high temperatures (10–1000K) through nanoindentation tests. We report the effects of increase of temperature on the nanoindentation process (Fig 3) like modifying dislocation densities and material hardness, in agreement with reported experimental measurements (Fig 4.). Our results suggest that [001] dislocation junctions are responsible for high-temperature material mechanical stability. Finally, we will present results for the nanoindentation test of irradiated Mo samples.

Neutron irradiation

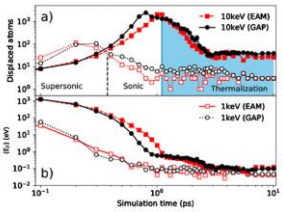


Fig 1. Number of displaced atoms as a function of the simulation time, where re-crystallization occurs during the thermalization phase.

Nanoindentation test

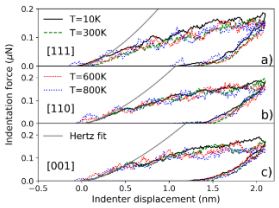


Fig 3. P– h curve of the nanoindentation of crystalline Mo for the [111] in (a), [110] in (b), and [001] in (c) crystal orientations.

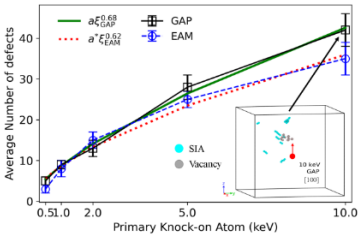


Fig 2. Total number of defects as a function of the PKA.

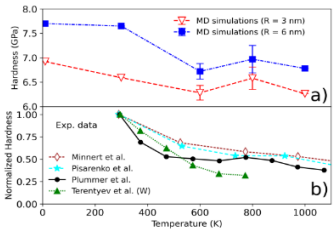


Fig 4. Hardness as a function of temperature for the [100] orientation

References

[1] F. J. Dominguez et al., Modelling Simul. Mater. Sci. Eng. **29**, 055001 (2021).

[2] F. J. Dominguez et al., Materials Science & Engineering A 826, 141912 (2021).

Modeling of the behaviour of materials under irradiation

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

Machine Learning for Atomistic Materials Science

Alexandra M. GORYAEVA[1], Tom D. SWINBURNE[2], Clovis LAPOINTE[1], Jacopo BAIMA[1], Julien DÉRÈS[1], Mihai-Cosmin MARINICA[1]

[1]Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France. [2]CNRS, Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), Université Aix-Marseille, France

Abstract

I will present recent advances in atomistic material simulations by means of machine learning and data-driven approaches. Machine learning (ML) methods cannot fully replace traditional approaches in physics and/or materials science. The phase space in physics / materials science has a well defined structure and is too vast and complex to be described only by the inherent statistical correlations within the data points. To our knowledge, none of the current statistical methods alone, generically called Machine Learning and its subclass deep learning (DL), can provide a valuable alternative to the laws of physics. In order to provide reliable results in the field of physics, ML/DL should learn and be trained on logically coherent data provided by well established methods from the community of physics. Nevertheless, statistical methods trained on the physical data can be of great help when the traditional approaches are limited and/or their direct application is hindered by factors such as high computational cost. Multi-scale approaches in materials science face a traditional dichotomy in the choice of the atomistic force fields: robust, accurate and numerically expensive ab initio methods against less transferable but fast empirical methods. The ML methods propose a third avenue that allows control of the balance between the accuracy and numerical efficiency. Moreover, the ML-based vision of fundamental concepts in materials science, such as structural defects, can augment and revise traditional interpretations. In metals, the interaction and transformation of crystal defect networks gives rise to an extraordinarily diverse range of defect morphologies [1]. Using the recently developed package MiLaDy (Machine Learning Dynamics) [2]: (i) we redefine the concept of defects in materials science [3]; (ii) we provide reliable force fields for complex defects such as interstitial, dislocation loops, dislocations; (iii) we are able to explore the atomistic free energy landscape of point defects in metals with ab initio accuracy up to the melting temperature [4], and, finally, (iv) we are able to propose surrogate models that bypass the traditional approaches [5]. We exemplify and discuss in the framework of experimental findings the case of energetic landscape of defects in body centered and face centered cubic metals.

References

[1] K. Arakawa , M.-C. Marinica et al. Nature Mat. 19, 508(2020) ; R. Alexander et al. Phys. Rev. B 94, 024103 (2016).
[2] M.-C. Marinica, A. M. Goryaeva, T. D. Swinburne et al, MiLaDy - Machine Learning Dynamics, CEA Saclay, 2015-2021 ; A.M. Goryaeva, J.-B. Maillet, M.-C. Marinica. Comp. Mater. Sci. 166, 200 (2019).
[3] A. M. Goryaeva et al. Nature Commun. 11, 4691 (2020).
[4] C. Lapointe et al. (to be submitted). , T.D. Swinburne, M.-C. Marinica, Phys. Rev. Lett. 120, 135503 (2018).
[5] C. Lapointe, T. D. Swinburne et al. , Phys. Rev. Materials 4, 063802 (2020); F. Bruneval et al. J. Chem. Theory Comput. 16, 4399 (2020).

Modeling of the behaviour of materials under irradiation

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

Materials informatics of High Entropy alloys

Stefanos PAPANIKOLAOU

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland

Abstract

The identification of alloys with exceptional properties has recently become rather promising with the advance of single-phase concentrated solid solutions (commonly known as high entropy alloys), containing multiple elements at large (>15%) concentrations. However, the search and understanding of such alloys is rather challenging, due to the prohibitive size of the multi-dimensional elemental and configurational space, together with the complexity of annealing-driven short-range disorder [1, 2] that masks the origin of mechanical properties' excellence. Facing these challenges requires multiscale modeling methods (ab-initio, molecular dynamics, Monte Carlo) that may allow for the appropriate physical interpretations of alloy searches, together with new approaches [3, 4 , 6], inspired from data science and widely labeled as materials informatics, where microscale parameters that control mechanical deformation at large scale can be identified, and even learned, from statistical analysis of large amounts of data.Consequent statistical predictions may range in a wide gamut of applications, for understanding of elastic and plastic features of deformation in crystals. By using multiscale modeling and materials informatics, I will outline several results related to the search [6], classification [3, 4, 5] and understanding [7, 8] of concentrated solid solution alloys.

References

[1] Papanikolaou, S., 2018. Learning local, quenched disorder in plasticity and other crackling noise phenomena. npj Computational Materials, 4(1), pp.1-7.
[2] Papanikolaou, S., Cui, Y. and Ghoniem, N., 2017. Avalanches and plastic flow in crystal plasticity: an overview. Modelling and Simulation in Materials Science and Engineering, 26(1), p.013001.
[3] Frydrych, K., Karimi, K., Pecelerowicz, M., Alvarez, R., Dominguez-Gutiérrez, F.J., Rovaris, F. and Papanikolaou, S., 2021. Materials Informatics for Mechanical Deformation: A Review of Applications and Challenges.
[4] Papanikolaou, S. and Alava, M.J., 2021. Direct detection of plasticity onset through total-strain profile evolution. Physical Review Materials, 5(8), p.083602.
[5] Papanikolaou, S., 2020. Microstructural inelastic fingerprints and data-rich predictions of plasticity and damage in solids. Computational Mechanics, 66(1), pp.141-154.
[6] Papanikolaou, S. 2021. Iron-based Alloys Informatics: Choosing how to alloy based on ab-initio-based charge profiles (in preparation).
[7] A. Esfandiarpour, S. Papanikolaou, M. Alava, Edge dislocations in multi-component concentrated solid solutions: Beyond the traditional elastic depinning theory (to be submitted, Phys. Rev. Letters).
[8] A. Naghdi, A. Poisvert, R. Alvarez, A. Esfandiarpour, K. Karimi, P. Sobkowicz, M. Alava, S. Papanikolaou, Segregation effects in equiatomic NiCoCr due to thermal annealing: A hybrid Monte-Carlo, Molecular Dynamics Investigation.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Quantitative microscopy for multiscale modelling

Wade KARLSEN

VTT Technical Research Centre of Finland, P.O. Box 1000, FI-02044 VTT, Finland

Abstract
Modelling of the plastic behavior of irradiated materials used in nuclear reactors can be described by constitutive equations capturing the temperature and strain rate sensitivities. To reflect the microstructural context, the flow stress must be decomposed into its fundamental components associated with the microstructure features peculiar to the particular steels, such as carbides, the dislocation network, deformation confinement inside grains, and strain localization in cleared channels. The contribution of radiation defects can be accounted for using atomistic and dislocation dynamics results. The effect of radiation-induced solute clusters and faulted dislocation loops can be analyzed in detail in terms of the feater size, density and strength. The aforementioned process involves a number of equations involving various parameters. In order to conduct calculations on real and representative materials systems, a number of inputs are often needed, many of which require quantifications to be carried out on images collected by microscopy and microanalysis techniques. Souces of error in such microscopy approaches in turn can introduce false or incorrect values into a multiscale computation exercise. Quantitative microscopy and associated considerations are the focus of this communication.

At the VTT Centre for Nuclear Safety, hot cell facilities combined with analytical electron microscopy enable experiments to be carried out on radiactive neutron irradiated materials such as reactor pressure vessel steels, austenitic stainless steel and nickel based internals materials, and nuclear fuel claddings. When it comes to reactor pressure vessel steels, examples are given of microstructural features that that can be involved in influencing the fracture toughness of the materials, such as dislocations, second phase particles, and irradiation-induced clusters. In austenitic stainless steels, features of primary importance to the materials' susceptibility to irradiation-assisted stress corrosion cracking include clusters and dislocation loops, localized plasticity through channel deformation, radiation-induced matrix precipitates, and radiation-induced grain boundary segregation. In precipitation-hardenable Ni-base alloy, the precipitate population size and distribution plays and important role in their mechanical performance in irradiation stress corrosion cracking performance. Finally, when it comes to zirconium fuel cladding, the dislocation loop population and particular properties are an important feature in the creep properties

References
[1] Wade Karlsen, "The new VTT Centre for Nuclear Safety", Suomalaisen Ydintekniikan Päivät 2016 – SYP2016. http://www.ats-fns.fi/fi/syp2016/proceedings.
[2] W. Karlsen, A. Toivonen and P. Efsing, Cor. and Mat. Deg., 2021, 2, 248-274. https://doi.org/10.3390/cmd2020014
[3] M. Sauzay, K. Bavard, W. Karlsen, J. of Nuc. Mat., Vol. 406, Issue 1, 1 November 2010, Pages 152-165.
[4] K. R. Anderson, W. Karlsen, M. Ivanchenko, J. J. Carter, R. W. Smith, J. of Nuc. Mat. Vol. 513 (2019) 260-270.
[5]W. Karlsen, K. Dohi, T. Onchi, 13th Int. Con. on Env.Deg. of Mat. in Nuc. Power Sys. Whistler, B.C., Canada, August 19 - 23, 2007. Canadian Nuclear Society, CNS (2007), 12 s.
[6] A. Toivonen, P. Aaltonen, W. Karlsen, U. Ehrnstén, J-P. Massoud, J-M Boursier 6th Int. Sym. on Contribution of Materials Investigations to Improve the Safety and Performance of LWRs. Fontevraud 6. Proceedings. Volume 1. Fontevraud Royal Abbey, France, 18-22 Sept. 2006. French Nuclear Energy Society, SFEN (2006), 567-579.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

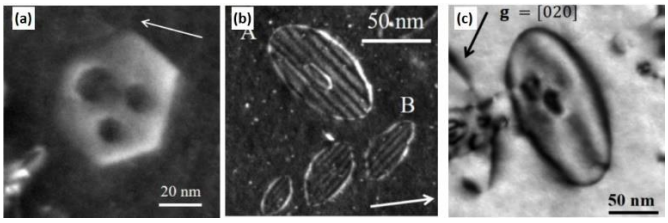
Solutes effects on the microstructural evolution of nickel base alloys as model alloy of austenitic steels

Kan MA[1,4], Brigitte DECAMPS[2], Thomas JOURDAN[1], Anna FRACZKIEWICZ[3], Frédéric PRIMA[4], Marie LOYER-PROST[1]

[1]Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette, France. [2] Laboratoire de Physique des 2 infinis Irène Joliot-Curie (IJCLab), Université Paris-Saclay, Orsay, France entre de Sciences Nucléaires et de Sciences de la Matière (CSNSM), CNRS-IN2P3- Université Paris-Sud, 101 Domaine de l'Université de Paris Sud, 91400 Orsay, France. [3] Institut de Recherche de Chimie Paris, CNRS UMR 8247–Chimie ParisTech, 11 rue Pierre et Marie Curie, Paris, 75005

Abstract

Austenitic Stainless Steels (ASSs) are foreseen as cladding material for next generation reactors even though their swelling under irradiation will limit the fuel burnup. Micro-additions of solute elements, such as chromium (Cr) and titanium (Ti), are known to efficiently reduce this swelling [1, 2] but the mechanism is still unexplained. To increase the swelling threshold, it is utmost important to get a better understanding of the mechanisms involved. Here we focus on the effect micro-additions (0,4% wt.) of an element (for example Ti and Cr) on the microstructure evolution of nickel at small irradiation dose. Nickel is considered as a model alloy for ASSs as they have the same crystallographic structure (face-centered cubic structure). Ni and its alloys were irradiated at high temperatures (450-510°C) by 2 MeV Ni^{2+} ions with a flux of 4 ± 0.8 x10^{11} ions/cm^2/s in a TEM using JANNuS-Orsay facility. The fluence was up to 10 ± 1.8 x10^{14} ions/cm^2 (0.7 dpa by SRIM-2013 and IRADINA [3]. The microstructure evolution of samples was recorded and analyzed. The drastic impact of solute elements on loop growth, morphology and nature will be detailed [4, 5]. The mechanisms involved will be discussed.



TEM micrographs of typical Frank loops in Ni (a), Ni-0,4Ti (b) and Ni-0,4Cr (c) irradiated at 450°C up to 0,7 dpa

References

[1] F.A.Garner, Radiation Damage in Austenitic Steels , volume 4, p. 33 (2012).
[2] A. Benkaddour et al. J Nucl. Mater. 217 (118-26). (1994).
[3] J.P Crocombette, et al. EPJ Nuclear Sciences & Technologies 5:7 (2019);
[4] K. Ma, et al., Materials Research Letters. 8 (2020) 201–207.
[5] K. Ma, et al., Acta Materialia. (2021) 116874.

Modeling of the behaviour of materials under irradiation

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

Nanoindentaion of ion-irradiated materials and thin films

Łukasz KURPASKA

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. Andrzeja Soltana 7, 05-400 Otwock, Poland

Abstract

In this study two subjects will be presented. First analyzes of the elastic-to-plastic transition during nanoindentation of polycrystalline iron (pristine and ion-irradiated) will be described. We conducted series of nanoindentation (by using Berkovich and spherical indenters) experiments and electron backscatter diffraction analysis and we investigated the initiation of plasticity by the appearance of the pop-in phenomenon in the loading curves. Numerous load–displacement curves were statistically analyzed to identify the occurrence of such events. According to our work, first pop-in results from plasticity initiation caused by homogeneous dislocation nucleation and requires shear stresses in the range of the theoretical strength of a defect free iron crystal [1]. The results also suggest that plasticity initiation in Fe specimen with preexisting dislocations is significantly affected by small amounts of interstitially dissolved atoms (such as C) that are segregated into the stress fields of dislocations, impeding their mobility (which is visible for ion irradiated sample). Another strong influence on the pop-in behavior may be the presence of grain boundaries, which can lead to large pop-ins at relatively high indentation loads. Obtain results suggest that the pop-in behavior appears to be a statistical process affected by interstitial atoms, dislocation density, grain boundaries, and surface roughness. Presented work is a part of the experimental campaign carried out at NCBJ in the frame of M4F project, and continued in the frame of NOMATEN.

Second part of the work will consist of the description of nanoindentation tests performed on alumina coatings [2]. In this study functional properties of a 1 µm thick Al2O3 coating, deposited on 316L stainless steel by Pulsed Laser Deposition (PLD), subjected to high energy ion irradiation were assessed. A comprehensive characterization combining Transmission Electron Microscopy and Grazing-Incidence X-ray Diffraction provided deep insight into the structure of the tested material at the nano- and micro-scale. Variation in the local atomic ordering of the irradiated zone at different doses was investigated using a reduced distribution function analysis obtained from electron diffraction data. Findings from nanoindentation measurements revealed a slight reduction in hardness of all irradiated layers. At the same time TEM examination indicated that the irradiated layer remained amorphous over the whole dpa range. No evidence of crystallization, void formation or element segregation was observed up to the highest implanted dose. Reported mechanical and structural findings were critically compared with each other pointing to the conclusion that under given irradiation conditions, over the whole range of doses used, alumina coatings exhibit excellent radiation resistance. Obtained data suggest that investigated material may be considered as a promising candidate for next-generation nuclear reactors, especially LFR-type, where high corrosion protection is one of the highest prerogatives to be met.

References

[1] F. Pohl, “Pop-in behavior and elastic-to-plastic transition of polycrystalline pure iron during sharp nanoindentation”, Scientific Reports 9 (2019) 15350.

[2] A. Zaborowska et al. “Absolute radiation tolerance of amorphous alumina coatings at room temperature”, Cremics International (2021), published.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Application of Calphad method (Zr Base alloys, carbides, etc)

Caroline TOFFOLON

Université Paris-Saclay, CEA, Service de Recherches Métallurgiques Appliquées, 91191 Gif-sur-Yvette cedex, France

Abstract
The so-called CALPHAD (CALculation of Phase Diagrams) method has shown its interest in the last 30 years for several alloy families such as steels, Ni-base, Ti-base alloys and in many fields of application.
This presentation aims at presenting how the CALPHAD method has been used for the development of useful tools for the study of phase transformations in fuel claddings used in Water Pressure Reactors.
Claddings containing the nuclear fuel in pressurized water reactors are made of zirconium alloys. It is of high interest to be able to predict the nature of the reactions with the surroundings (water), the precipitation or the dissolution of phases induced by the presence of alloying elements, but also to test new alloy compositions.
In a first part, the creation of thermodynamic database using the CALPHAD method will be presented. This method is an extensively used semi-empirical technique for phase modeling. It consists in describing the Gibbs energies of the different phases present in a system by adjusting parameters to fit the known experimental data and DFT calculations [1].
Then, results showing the interest of thermodynamic calculations to metallurgical studies of multi-component zirconium based alloys will be presented [2-3].
In a last part, it will be shown how thermodynamic databases, when linked to other modelling tools, can provide useful thermodynamic and/or metallurgical data [4].

References
[1] P. Lafaye *et al.*, "Experimental study, first principles calculations and thermodynamic modelling of the Cr-Fe-Nb-Sn-Zr quinary system for nuclear applications", Journal of Nuclear Materials, 544 (2021) 152692.
[2] J.-C. Brachet *et al.*, "Oxygen, Hygroden and Main Alloying Chemical Elements Partitioning Upon Alpha-Beta phase Transformation in Zirconium Alloys", Solid State Phenomena **172-174** (2011) 753-759.
[3] C. Toffolon-Masclet *et al.* "Contribution of Thermodynamic Calculations to Metallurgical Studies of Multi-Component Zirconium based Alloys", Journal of ASTM International **5** N°7 (2008) 1-21.
[4] C. Toffolon-Masclet, C. Desgranges, C. Corvalan and J.-C. Brachet, "Simulation of the beta to alpha (O) phase transformation due to oxygen diffusion during high temperature oxidation of zirconium alloys", Solid State Phenomena 172-174 (2011) 652-657.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Corrosion modelling: Estimation KINetics OXidation code

Laure MARTINELLI[1], Caroline TOFFOLON[2], Clara DESGRANGES[3], Florence LEQUIEN[1], Benoit MAZERES[4], Maylise NASTAR[5], Daniel MONCEAU[6]

[1] Université Paris-Saclay, CEA, Service de la Corrosion et du Comportement des Matériaux dans leur Environnement, 91191, Gif-sur-Yvette, France. [2] Université Paris-Saclay, CEA, Service de Recherches Métallurgiques Appliquées, 91191, Gif-sur-Yvette, France. [3] Safran-Tech, rue des jeunes bois, Châteaufort, CS80112, 78772, Magny les hameaux, France. [4] Communauté urbaine Grand Paris Seine et Oise. [5] Université Paris-Saclay, CEA, Service de Recherches Métallurgiques Physiques, 91191, Gif-sur-Yvette, France. [6] CIRIMAT, CNRS, INPT, UPS, ENSIACET, Universite´ de Toulouse, Toulouse Cedex 4, France

Abstract

EKINOX code (EstimationKINeticsOXidation) has been developed to simulate oxide scale growth kinetics as well as the evolution of the substrate during the high temperature oxidation. It consists in solving a set of diffusion equations with moving interface conditions on metal/oxide and oxide/environment interfaces in a 1D discretised space. The classical pseudo stationary state hypothesis is not postulated which enables to calculated the kinetics of transient states. This numerical tool has been adapted to perform simulations of the high temperature oxidation of Zr alloys on one hand and (Fe)-Ni-Cr alloys on the other hand. For Zr alloy application, the code had been coupled with a CALPHAD thermodynamics database. The objective was to predict the oxygen concentration profile and the growth kinetics of oxide scale and Zr(O) metallic phase in the 600µm thick cladding wall during a Loss Of Coolant Accident scenario. Simulations performed with the EKINOX-Zr code had been for example used to study the impact of H concentration within the cladding on the residual ductility of the cladding after a LOCA scenario. For (Fe)-Ni-Cr alloy application, the main objective was to simulate the evolution of vacancy and Cr and Ni concentrations in the alloy during high temperature oxidation. The elimination and creation of the vacancies by sources and sinks in the alloy was also taken into account in the calculations. Simulations had been used to study, chromia scale growth, Cr depletion profile and the risk of voids formation in the alloy by local vacancy oversaturation phenomena.

References

Ekinox Fe-Ni-Cr:
L. Bataillou et al, Corr Sc 136 (2018) 148–160.
C. Desgranges et al, Oxid Met (2013) 79:93-105.
N. Bertrand et al, Mat Sc For vol. 595 -598 (2008).
C. Desgranges et al, Mat Sc For Vols. 461-464 (2004).
Ekinox Zr:
Toffolon et al, ZIRCONIUM IN THE NUCLEAR INDUSTRY: 19TH INTERNATIONAL SYMPOSIUM, ed. A. T. Motta and S. K. Yagnik (West Conshohocken, PA: ASTM International, 2021).
B.Mazères et al, Corr Sc 103 (2016) 10–19.
B.Mazères et al, Oxid Met (2013) 79:121–133.
C. Corvalán et al, J Nucl Mat 400 (2010) 196–204.

Modeling of the behaviour of materials under irradiation

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

Modeling of the behaviour of materials under irradiation

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

Abstracts of the communications
(Thursday, November 18, Parts 3 & 4)

Modeling of the behaviour of materials under irradiation

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

Modeling of the behaviour of materials under irradiation

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

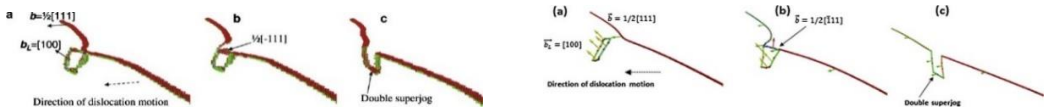
Dislocation interactions with radiation-induced loops in metals using Dislocation Dynamics simulations

Laurent DUPUY, Fabien ONIMUS

Université Paris-Saclay, CEA, Service de Recherches Métallurgiques Appliquées, 91191 Gif-sur-Yvette cedex, France

Abstract

Material science has clearly established a link between nanometric radiation-induced defects and various macroscopic material ageing phenomena, such as irradiation hardening, strain localization or embrittlement. Building *quantitative* models is nevertheless an active research field: on the one hand, molecular dynamics studies enlighten the wealth of the interactions between individual dislocations with radiation-induced defects, such as dislocation loops, stacking-fault tetrahedral, cavities, bubbles, precipitates or C15 clusters [1-2]. On the other hand, modelling plasticity at the grain level necessarily involves the motion of a large amount of dislocations and dislocation-defect interactions, which is out-of-reach of molecular dynamics simulations, and is rather the realm of dislocation dynamics simulations [3-4]. This multiscale approach raises nevertheless a series of questions: how accurate are dislocation dynamics simulations when it comes to handle nanometer-sized objects such as radiation-induced defects? Is elasticity still relevant at such scales? What is the minimal set of parameters needed from atomic scales? Beyond input parameters: are there missing features or mechanisms? This communication will address these questions, with a particular focus, on dislocation interactions with radiation-induced loops in iron and zirconium metals [5-6]. Detailed comparisons between molecular dynamics simulations and dislocation dynamics simulations are presented and motivate the concept of *atomistically informed dislocation dynamics* simulations [7]. As an experimental validation, we show how to use these simulations to understand *in situ* experiments on irradiated materials [8].



Interaction between an edge dislocation and a {100} loop in iron. Left : molecular dynamics simulation (courtesy D. Terentyev). Right : dislocation dynamics simulation

References

[1] Bacon, D. J., Osetsky, Y., & Rodney, D. (2009). Dislocation–obstacle interactions at the atomic level. Dislocations in solids, 15, 1-90.

[2] Dérès, J., Proville, L., & Marinica, M. C. (2015). Dislocation depinning from nano-sized irradiation defects in a bcc iron model. Acta Materialia, 99, 99-105.

[3] Nogaret, T., Rodney, D., Fivel, M., & Robertson, C. (2008). Clear band formation simulated by dislocation dynamics: Role of helical turns and pile-ups. Journal of Nuclear Materials, 380(1-3), 22-29.

[4] Marian, J., Fitzgerald, S., & Po, G. (2020). Discrete dislocation dynamics simulations of irradiation hardening in nuclear materials. Handbook of Materials Modeling: Applications: Current and Emerging Materials, 2243-2271.

[5] Shi, X. J., Dupuy, L., Devincre, B., Terentyev, D., & Vincent, L. (2015). Interaction of< 1 0 0> dislocation loops with dislocations studied by dislocation dynamics in α-iron. Journal of Nuclear Materials, 460, 37-43.

[6] Drouet, J., Dupuy, L., Onimus, F., Mompiou, F., Perusin, S., & Ambard, A. (2014). Dislocation dynamics simulations of interactions between gliding dislocations and radiation induced prismatic loops in zirconium. Journal of Nuclear Materials, 449(1-3), 252-262.

[7] Martinez, E., Marian, J., Arsenlis, A., Victoria, M., & Perlado, J. M. (2008). Atomistically informed dislocation dynamics in fcc crystals. Journal of the Mechanics and Physics of Solids, 56(3), 869-895.

[8] Drouet, J., Dupuy, L., Onimus, F., & Mompiou, F. (2016). A direct comparison between in-situ transmission electron microscopy observations and Dislocation Dynamics simulations of interaction between dislocation and irradiation induced loop in a zirconium alloy. Scripta Materialia, 119, 71-75.

Modeling of the behaviour of materials under irradiation

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

Multiscale modelling of plasticity with discrete dislocation dynamics

Mikko ALAVA

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. Andrzeja Soltana 7, 05-400 Otwock, Poland

Abstract

Discrete Dislocation Dynamics (DDD) models plasticity in a context where numerical challenge competes with physical detail but one gets rewarded by „real material behavior" compared to what happens on scales accessible to eg. Molecular Dynamics. DDD follows an ensemble of dislocations interacting with the „matrix" of the background material. There are many approaches of how to solve this problem numerically in general and how to handshake the microscopic information from MD and smaller spatial and temporal scales. In this talk, I review what happens in the case of coherent precipitates. The inclusion of the relevant detail needs a multiscale approach [1] but can then be used to mimic the effects of radiation damage [2]. What merges from this modelling effort is a complete picture of how precipitates and other pinning defects modify the yield stress on micron scales [3,4] and why. I will review approaches to fight the numerical challenges met by High-Performance Computing, and how to combine DDD to Machine Learning approaches [5].

References

[1] A. Lehtinen et al. Phys. Rev. E93, 013309 (2016).
[2] A. Lehtinen et al. Sci. Rep. 8, 1 (2018).
[3] H. Salmenjoki, L. Laurson, and M.J. Alava, Phys. Rev. Mat. 4, 083602 (2020).
[4] H. Salmenjoki, L. Laurson, and M.J. Alava, Phys. Rev. Mat. 5, 073601 (2021).
[5] H. Salmenjoki, L. Laurson, and M.J. Alava, Materials Theory 4, 5 (2020).

Modeling of the behaviour of materials under irradiation

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

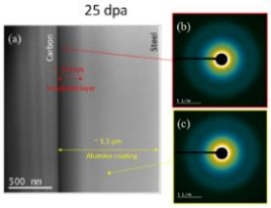
Effects of radiation and temperature on performance of PLD-grown alumina coatings dedicated for LFR

Agata ZABOROWSKA[a)], Łukasz KURPASKA[a)], Mélanie CLOZEL[a)], Edyta WYSZKOWSKA[a)], Katarzyna MULEWSKA[a)], E. Jaco OLIVIER[b)], Jacques Herman O'CONNELL[b)], Fabio DI FONZO[c)], Witold CHROMIŃSKI [a,d)], Maciej ZIELIŃSKI [a)], Alexander AZAROV[a,e)], Iwona JÓŹWIK[a,f)], Malgorzata FRELEK-KOZAK[a)], Ryszard DIDUSZKO[f)],

[a)]National Center for Nuclear Research, Poland; [b)]Nelson Mandela University, South Africa; [c)]Istituto Italiano di Tecnologia, Italy; [d)]Warsaw University of Technology, Poland; [e)]University of Oslo, Norway, [f)]Łukasiewicz Research Network - Institute of Microelectronics and Photonics

Abstract

Lead-cooled fast reactor (LFR) is one of Generation IV concepts, allowing to close the fuel cycle and thus to reduce the uranium consumption and to limit the volume of high-level wastes for disposal [1]. The main drawback of the advanced lead or lead–bismuth eutectic (LBE) cooled energy systems is the issue related to corrosion degradation of structural materials exposed to the heavy liquid metal [2]. One of the corrosion mitigation strategies consists in deposition of an external coating on the steel substrate. The leading candidate for the coating material is alumina. In the past decade, a growing interest of the nuclear community in PLD-grown alumina coatings have been observed [3–7]. Available literature data prove that PLD-grown Al2O3 coatings show excellent corrosion resistance in the range of environments (up to 10 000 h, flowing/stagnant Pb/Pb-55Bi, 10-3-10-8 wt.%O2) and exhibit a number of features desirable for nuclear applications [3-7]. Presented work is a part of the ongoing research on this topic. Performed studies focus on the influence of high temperature and radiation damage on the coating properties. To determine the effect of the anticipated service conditions (up to 550 °C and 200 dpa) on materials performance a series of room and high temperature tests were performed. 1 µm PLD-grown amorphous Al_2O_3 coatings deposited at room temperature were ion irradiated. Comprehensive post-irradiation characterization comprising microstructural and mechanical analysis was performed using X-ray diffraction, transmission electron microscopy and nanoindentation. To study the evolution of the coating under high temperature, in situ nanoindentation (up to 650 °C) and X-ray diffraction (up to 1100 °C) measurements were carried out. Overall, the results obtained so far are very promising and show that the system retains its integrity under the conditions investigated.



(a) HAADF-STEM cross-sectional micrograph showing the alumina coating after 25 dpa ion irradiation (1.2 MeV Au^+) and corresponding DP's of: (b) irradiated layer and (c) unmodified coating volume

References

[1] P. Lorusso et al., GEN-IV LFR development: Status & perspectives. Prog. Nucl. Energy (2018).
[2] J.B. Vogt, I.P. Serre, A review of the surface modifications for corrosion mitigation of steels in lead and LBE, Coatings (2021) doi:10.3390/coatings11010053.
[3] F.G. Ferré et al., Corrosion and radiation resistant nanoceramic coatings for lead fast reactors, Corros. Sci. (2017) doi:10.1016/j.corsci.2017.05.011.
[4] F.G. Ferré et al., Radiation endurance in Al2O3nanoceramics, Sci. Rep. (2016) doi:10.1038/srep33478.
[5] A. Zaborowska et al., Absolute radiation tolerance of amorphous alumina coatings at room temperature, Ceram. Int. (2021) doi:10.1016/j.ceramint.2021.09.013.
[6] D. Iadicicco et al., Multifunctional nanoceramic coatings for future generation nuclear systems, Fusion Eng. Des. (2019) doi:10.1016/j.fusengdes.2019.03.004.
[7] F.G. Ferré et al., Advanced Al2O3 coatings for high temperature operation of steels in heavy liquid metals: a preliminary study. Corros. Sci. (2013) https://doi.org/10.1016/j.corsci.2013.07.0"9.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Polycristalline modelling of the behavior of neutron-irradiated recrystallized Zr alloys during strain path change tests

Fabien ONIMUS

Université Paris-Saclay, CEA, Service de Recherches Métallurgiques Appliquées, 91191 Gif-sur-Yvette cedex, France

Abstract

During normal operating conditions, zirconium alloy nuclear fuel cladding tubes experience various biaxial loadings with complex strain path histories. Experiments have been conducted on neutron-irradiated thin cladding tubes in order to study the response to changes in the loading path. These tests consist of alternate internal pressure tests and axial tensile tests [1]. During the internal pressure test steps, the flow stress exhibits significant cyclic strain softening, while axial tensile tests exhibit a smaller degree of cyclic strain softening. TEM analyses of the tested samples have revealed that the observed mechanical behavior can be attributed to clearing of irradiation-induced defect by gliding dislocations. The cyclic strain softening observed for internal pressure tests is due to clearing of defects by dislocations gliding in the basal planes [2]. The smaller degree of cyclic strain softening in tensile tests is due to clearing of defects by dislocations gliding in the prismatic and pyramidal planes. A polycrystalline model [3,4] has been developed to simulate these tests. This model is able to reproduce many features of the complex behavior of the material and provides a better understanding of the role of the clearing of defects and the contribution of kinematic hardening on the behavior of neutron-irradiated recrystallized zirconium alloys.

References

[1] Onimus, F., Bono, M., Garnier, J., Soniak-Defresne, A., Limon, R., Gilbon, D., Bourlier, F., Ambard, A., 2018. Strain-Path Change Tests and Physically Based Polycrystalline Modeling of the Behavior of Recrystallized Zirconium Alloys. Zirconium in the Nuclear Industry: 18th International Symposium, ASTM International, ASTM STP 1597, 180–213.
[2] Onimus, F., Monnet, I., Béchade, J.., Prioul, C., Pilvin, P., 2004. A statistical TEM investigation of dislocation channeling mechanism in neutron irradiated zirconium alloys. Journal of Nuclear Materials 328, 165–179.
[3] Cailletaud, G., 1992. A micromechanical approach to inelastic behaviour of metals. International Journal of Plasticity 8, 55–73.
[4] Onimus, F., Béchade, J.-L., 2009. A polycrystalline modeling of the mechanical behavior of neutron irradiated zirconium alloys. Journal of Nuclear Materials 384, 163–174.

Modeling of the behaviour of materials under irradiation

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

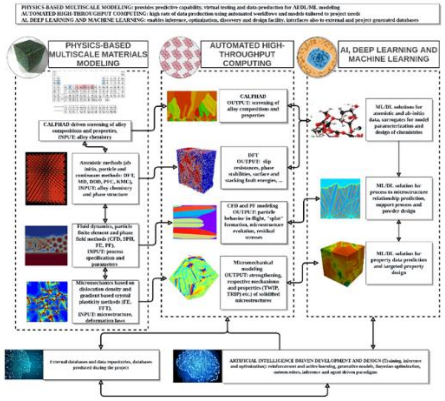
Utilizing micromechanical modeling aspart of the ICME workflow for irradiated materials

Matti LINDROOS, Anssi LAUKKANEN, Wade KARLSEN, Z. QUE, Sicong REN, Tom ANDERSSON, Tatu PINOMAA, Sami MAJANIEMI

VTT Technical Research Centre of Finland, P.O. Box 1000, FI-02044 VTT, Finland

Abstract

Integrated computational materials engineering (ICME) brings together multi-scale modeling, advanced experimental activities and recent machine learning, artificial intelligence and material discovery. In physics based modeling and data-driven methods, micromechanical descriptions of material behavior is at the core of ICME due to its capability to present link microstructure to properties and finally to performance. Various approaches such as MD,DD,DFT,PF,KMC are much appreciated in terms of understanding the role of irradiation to the performance (e.g. fracture susceptibility) of nuclear materials. The length and time scales in addition to the computational cost often become restrictive in terms of availing predictions covering polycrystal materials. The role of micromechanics, often described with crystal plasticity, is to enable analysis of large polycrystalline microstructures in terms of mechanical response, either under arbitrary deformation or aging phenomena. The description of the material behavior (constitutive relations) much relies on the understood phenomena at very fine scales, for example, dislocation mechanism, defect structures, evolution of solute segregation, and nucleation of fracture. On the other hand, the quality of characterization data is reflected directly on the inputted representativenes of computational microstructures of its local features. As such, the effectiveness of micromechanical predictions then depends much on the input data provided by multi-scale modeling techniques and usable experimental data. ML/AI approaches provide additional feedback of understanding experimental datasets, however, most importantly when physics-based models input data to ML/DL/AI, the prediction capability of high-throughput models is affected to an extent. In this communation, we discuss the bridging and use of other modeling techniques jointly with micromechanical modeling, emphasis on crystal plasticity and couplings with phase field, O/KMC and machine learning [1-3].



References

[1] A. Laukkanen and T. Pinomaa and T. Andersson and M. Lindroos and I. Yashchuck and T. Suhonen, Data-driven optimization of metal additive manufacturing solutions, In Euro PM2019 Congress and Exhibition, EPMA, pp. 1-6.

[2] T. Pinomaa and M. Lindroos and P. Jreidini and Matias Haapalehto and K. Ammar and Lei Wang and A. Laukkanen and and S. Forest and N. Provatas, Multiscale analysis of crystalline defect formation in rapid solidification of pure aluminium and aluminium-copper alloys, Philosophical Transactions A, Accepted 2021.

[3] M. Lindroos and T. Pinomaa and K. Ammar and A. Laukkanen and and S. Forest and N. Provatas, Dislocation density in cellular rapid solidification using phase field modeling and crystal plasticity, International Journal of Plasticity, Accepted 2021.

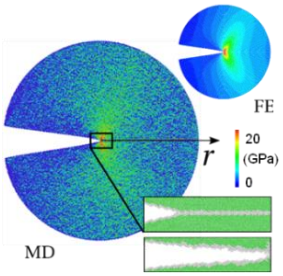
Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Interface intergranular fracture prediction using multi-scale simulations

Bertrand SICAUD[1,2], Laurent Van BRUTZEL[1], Maxime SAUZAY[2]

[1] Université Paris-Saclay, CEA, Service de la Corrosion et du Comportement des Matériaux dans leur Environnement, France. [2] Université Paris-Saclay, CEA, Service de Recherches Métallurgiques Appliquées (SRMA), France

Abstract
Irradiation assisted stress corrosion cracking (IASCC) of austenitic stainless steels is reported in internals components of pressurized water reactor vessels in nuclear power plants. The underlying mechanisms of IASCC are not yet fully understood, because many complex synergetic mechanisms are involved. Beside some efforts to develop empirical models, it is necessary to develop more physical-based prediction models. However, it has been demonstrated that localized plasticity in the form of clear bands triggers intergranular cracking in irradiated 316L stainless steel exposed to either inert or water environments. Preferential oxidation at grain boundaries further constitutes a major influence on stress corrosion cracking in nickel-based alloys. In this context, simulations at two different length scales are performed to provide physical insights in order to enhance the prediction of crack initiation. At the atomic scale, molecular dynamics simulations using empirical potential on pure nickel show the influence of stress multiaxiality over the behavior of various bi-crystals prone to either dislocation nucleation at grain boundary or grain boundary decohesion. At the grain scale, finite element computations using crystalline elastoplascity are used for the assessment of stress concentrations at various impacts of slip bands (and clear bands) onto grain boundaries. Two different multiscale approaches are subsequently carried out to propose a prediction of intergranular fracture initiation in the context of a coupled criterion (stress and energy coupled equation) for crack initiation: 1) a bottom-up approach, chaining atomistic grain boundary mechanical parameters to a semi-analytical finite element-based model, 2) a top-down approach, applying displacement fields extracted from finite element computations of slip bands impacts on various GB configurations in molecular dynamics. The coherency of the two approaches seems to validate the use of a coupled criterion for crack initiation at this scale. Predictions agree with experimental results and underline the influence of grain size on IASCC.



Top-down approach illustrated in the case of the Σ5 [031] grain boundary at a remoted stress of 28.7 MPa. Atomic stress field (MD) compared to the finite element computed stress field (FE). During the relaxation process of the deformed configuration in the atomic simulation, crack initiates (two bottom figures).

References
B. Sicaud, (2020). Multiscale simulations of intergranular fracture initiation in face-centered cubicmetals and alloys: influence of the localised plastic slip deformation. PhD thesis, Sorbonne Université.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Modelling of inhomogeneous fracture toughness behavior of irradiated reactor pressure vessel steels

Sebastian LINDQVIST

VTT Technical Research Centre of Finland, P.O. Box 1000, FI-02044 VTT, Finland

Abstract

Modelling of fracture toughness in the ductile-to-brittle transition (DBTT) region is challenging due to interaction occurring on different scales to create the weakest link. Fracture toughness has a stochastic nature in the transition region complicated further by macroscopic inhomogeneities. Modelling in the DBTT region is a balancing act between engineering applicability and micro mechanistic description of the fracture process. Master Curve offers an engineering solution to the problem with a micro-mechanistic description of the statistical behavior in the DBTT region and an empirical temperature dependence, both being characteristic for ferritic steels. Recently, an inhomogeneity analysis has been implemented to the ASTM E1921 standard utilizing the Master Curve method, but guidelines do not offer advice for applying the new methods to irradiated materials with varying fluence. The goal is to describe some practical ways to model inhomogeneous material behavior in the DBTT region with the Master Curve model by accounting for different levels of irradiation embrittlement.

References

[1] Wallin K. Assessment of master curve material inhomogeneity using small data sets. PVP2018-84297. Am Soc Mech Eng Press Vessel Pip Div PVP 2018;PVP2018:1–10. https://doi.org/10.1115/PVP201884297.

[2] Wallin K, Nevasmaa P, Laukkanen A, Planman T. Master Curve analysis of inhomogeneous ferritic steels. Eng Fract Mech 2004;71:2329–46. https://doi.org/10.1016/j.engfracmech.2004.01.010.

[3] ASTM E1921-20. Standard Test Method for Determination of Reference Temperature, To, for Ferritic Steels in the Transition Range. ASTM Int 2020.

[4] Lindqvist S, Ahonen M, Lydman J, Arffman P, Hänninen H. A crack-location correction for T0 analysis of an Alloy 52 dissimilar metal weld. Eng Fract Mech 2019;214:320–34. https://doi.org/10.1016/j.engfracmech.2019.03.001.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Fracture behavior of austenitic stainless steels used for Pressurized Water Reactors (PWR) internals structures

Jérémy HURE, Benoît TANGUY, Jean-Michel SCHERER, Cédric SÉNAC

Université Paris-Saclay, CEA, Service d'Etudes des Matériaux Irradiés, 91191 Gif-sur-Yvette cedex, France

Abstract

Austenitic stainless steels are used for the internals structures of Pressurized Water Reactors (PWR) owing to their good mechanical properties and resistance to corrosion. In PWRs currently in service in France, baffle and former plates are made of Solution-Annealed 304(L) while Baffle-to-Former Bolts (BFB) are made of Cold-Worked 316(L). The internals structures are subjected to harsh conditions including high temperature (~300°C), contact with PWR aqueous environment and very high irradiation dose (up to 80dpa). High temperature neutron irradiation leads to drastic microstructural changes, mostly Frank loops, which in turn induces strong evolutions of mechanical and fracture properties [1]. The main failure mode of austenitic stainless steels at PWR operating temperature is ductile through internal void growth to coalescence mechanism. Irradiation affects fracture toughness – measuring the energy required for crack to propagate – up to a tenfold decrease [2], associated with unstable crack propagation. In addition, austenitic stainless steels become susceptible to a degradation phenomenon called Irradiation Assisted Stress Corrosion Cracking (IASCC), leading to failures of baffle-to-former bolts through the initiation and propagation of intergranular cracks [3]. Macroscopic and / or engineering models aiming at predicting these failure modes are proposed in the literature, but refined modelling at the relevant scale is still lacking. This communication thus focuses on the numerical models and tools developed to assess fracture behaviour of austenitic stainless steels at the polycrystalline scale. Such scale is relevant for IASCC that occurs through intergranular cracking, but also for ductile fracture where voids are mostly smaller than the grain size. In a first part, physically based crystal plasticity constitutive equations aiming at modelling grain scale plasticity of austenitic stainless steels are presented, including extensions to account for irradiation defects [4]. Calibration of the parameters of the model through dedicated experiments on single crystals is discussed. In a second part, the extension of the constitutive equations to account for the presence of voids is described [5], and the model is validated by comparisons to porous single crystal unit cells simulations performed using AMITEX_FFTP solver. Numerical implementation of these constitutive equations within the MFront code generator is briefly discussed. In a final part, two numerical simulations on structures using these constitutive equations are detailed. The first one corresponds to FFT-based simulations of polycrystalline aggregates in order to assess intergranular stresses in the context of IASCC modelling, incorporating a model to account for the effect of grain boundaries on local hardening [6]. The second one corresponds to ductile tearing of polycrystalline aggregates in the context of ductile fracture modelling.

References

[1] Was, G.S. 2007. Fundamentals of Radiation Materials Science: Metals and Alloys. Springer.
[2] Chopra, O.K., & Rao, A.S. 2011. A review of irradiation effects on LWR core internal materials: Neutron embrittlement. J. Nuc. Mat., 412, 195–208.
[3] Chopra, O.K., & Rao, A.S. 2011. A review of irradiation effects on LWR core internal materials: IASCC susceptibility and crack growth rates of austenitic stainless steels. J. Nuc. Mat., 409, 235–256.
[4] Hure, J., El Shawish, S., Cizelj, L., & Tanguy, B. 2016. Intergranular stress distributions in polycrystalline aggregates of irradiated stainless steel. J. Nuc. Mat., 476, 231 – 242.
[5] Scherer, J.M., Besson, J., Forest, S., Hure, J. & Tanguy, B. 2021. A strain gradient plasticity model of porous single crystal ductile fracture. J. Mech. Phys. Sol., 156, 104606.
[6] Liang, D., Hure, J., Courcelle, A., El Shawish, S., & Tanguy, B. 2021. A micromechanical analysis of intergranular stress corrosion cracking of an irradiated stainless steel. Acta Mat., 204, 116482.

Modeling of the behaviour of materials under irradiation

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

Study and modelling of tritium trapping in fusion relevant materials

Etienne A. HODILLE[1], Rémi DELAPORTE-MATHURIN[1,2], James DARK[1,2], Jonathan MOUGENOT[2], Yann CHARLES[2], Andree DE BACKER[2], Charlotte BECQUART[3], Jean DENIS[4], Yves FERRO[4], Christian GRISOLIA[1]

[1]CEA IRFM, F-13108 Saint Paul Lez Durance, Cadarache France. [2]Université Sorbonne Paris Nord, LSPM, CNRS, UPR 3407, F-93439, Villetaneusse, France. [3]Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207, UMET, F-59000 Lille, France. [4]Aix Marseille Université, CNRS, PIIM UMR 7345, 13397 Marseille, France

Abstract

Trapping, diffusion and desorption of hydrogen isotopes (HI) in plasma facing components (PFC) are key issues for the development of fusion as an energy source. First, safety regulations limit the total inventory of tritium in ITER vessel to 700 g. In addition, the inventory of HI and their desorption into the plasma can negatively affect the overall plasma control. Furthermore, tritium can permeate from the plasma exposed surfaces to the cooling loop and spread in them.Thus, these phenomona have to be accurately predicted to allow a safe and reliable operation of a fusion reactor. For that purpose, we developped thermo-kinetic models based on macroscopic rate equations (MRE) that couples diffusion of mobile HI in the materials with trapping at defects. In this communication, we present a tool called MHIMS [1,2] (Migration of Hydrogen Isotopes in MaterialS) developped at the CEA/IRFM which can be used in a multi-scale modelling framework regarding the H/metal interactions [3, 4]. In this multi-scale modelling framework, the model implemented in MHIMS takes input from atomistic calculation method such as DFT (density functional theory) which provides parametrizations for the H/material interactions. In particular, the diffusion, the trapping at defects (vacancy, vacancy clusters or dislocations ...) and the desorption/absorption kinetics are parametrized from DFT calculations [5,6,7]. This DFT-parametrized model can then be compared to experimental results among which the Thermal Desorption Spectrometry (TDS) is one of the most important one. It consists in loading a material sample with HI, heating it with a controlled temperature evolution and record the D desorption flux obtained. This method can also be coupled with profilometry methods such as Nuclear Reaction Analysis (NRA). After the model is experimentally verified, it can be used to simulate the retention, outgassing and permeation of fuel during realistic tokamak cycles that will be done in ITER. To simulate the migration of His during such cycles in the complex geometry of the actively cooled PFCs, a mutli-dimensional finite element code called FESTIM [8] is used. It allows to predict the evolution of the HI concentration field in PFCs for various exposure conditions during ITER futur plasma as well as the evolution of the amount of fuel release to the cooling system.

References

[1] E.A. Hodille et al, J. Nucl. Mater. 467 (2015) 424-431.
[2] E. A. Hodille et al, Nucl. Fusion 57 (2017) 056002.
[3] E. A. Hodille et al, Phys. Scr. T167 (2016) 014011 .
[4] E. A. Hodille et al, Nucl. Fusion 57 (2017) 076019.
[5] Fernandez et al, Acta Mater. 94 (2015) 307-318.
[6] Hou et al, Nature Mater. 18 (2019) 833-839.
[7] Ajmalghan et al, Nuc. Fusion 59 (2019) 106022.
[8] R. Delaporte-Mathurin et al, Nucl. Mater. Energ. 21 (2019) 100706.

Modeling of the behaviour of materials under irradiation

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

Unconventional application of microscopic techniques in analysis of irradiated materials

Iwona JÓŹWIK[a,b], Jacek JAGIELSKI[b,c], Marcin S. ZIELINSKI [d], Libor KOVARIK[e], Bruce AREY[e],

[a] NOMATEN Centre of Excellence, NOMATEN MAB, National Centre for Nuclear Research, Department of Physics, 7th A. Soltana Str., Świerk-Otwock, Poland; [b] Lukasiewicz Research Network – Institute of Microelectronics and Photonics, Al. Lotników 32/46, Warsaw, Poland; [c] National Centre for Nuclear Research, Department of Physics, 7th A. Soltana Str., Świerk-Otwock, Poland; [d] Attolight AG, EPFL Innovation Park/Bldg. D, 1015 Lausanne, Switzerland; [e] Pacific Northwest National Laboratory, Richland, WA 99352, USA

Abstract

The investigation of the damage accumulation process in irradiated solids is one of the key issues of nuclear engineering. The development of predictive models for the behavior of materials in nuclear installations requires detailed understanding of the mechanisms leading to structural transformations and, consequently, changes in their functional properties. In general the study of the damage accumulation process involves three main aspects: (i) the identification of the type of defects that are created at the various stages of the damaging process, (ii) the quantitative determination of the damage level and (iii) the modelling of the damage accumulation buildup. Various experimental and simulation tools may be used to achieve the goals listed above. The most reliable technique for the determination of the defect structure is certainly transmission electron microscopy (TEM), whereas the quantitative analysis of the damage and stress levels is generally done using Rutherford backscattering/channeling (RBS/C) and X-ray diffraction (XRD).

In this communication, the methods of ion damage studies in $MgAl_2O_4$, $Gd_2Ti_2O_7$, $SrTiO_3$ and semiconductors, based on low voltage scanning electron microscopy (SEM) and cathodoluminescence (CL), as well as transmission electron microscopy in non-conventional application will be presented. The results imply that the low-energy CL is more sensitive to low damage levels as compared to RBS/C and it can be efficiently used as a complementary tool showing new perspectives in the damage accumulation studies in single- and polycrystalline materials even for low ion doses [1, 2]. Another example is that TEM analysis may deliver the information on strain in the irradiated material, when the system is brought to non-standard operating conditions [3]. Special attention will be focused on the application of scanning electron microscopy at low beam acceleration voltages (low-kV SEM) to direct visualization of ion-irradiated damage in semiconductors. The mechanism of image contrast formation is based on local changes of material resistivity leading to changes of surface potential under electron beam, and it was named by the authors as Damage-Induced Voltage Alteration contrast (DIVA) [4-6].

References

[1] I. Jozwik, M.S. Zielinski, A. Azarov, R. Ratajczak, C. Mieszczynski, A. Stonert, J. Jagielski, Nuclear Inst. and Methods in Physics Research B 435 (2018) 290-295.

[2] I. Jozwik, J. Jagielski, G. Gawlik, P. Jozwik, R. Ratajczak, G. Panczer, N. Moncoffre, A. Wajler, A. Sidorowicz, L. Thome, Phys.Chem.Minerals 43(6) (2016) 439-445.

[3] J. Jagielski, P. Jozwik, I. Jozwik-Biala, L. Kovarik, B. Arey, J. Gaca and W. Jiang, Radiation Effects and Defects in Solids, 168(6) (2013) 442.

[4] I. Jóźwik, E. Dąbrowska, A. Maląg, A. Barcz, ECS J. Solid State Sci. Technol. 6(7)(2017)415-417.

[5] I. Jozwik, A.Barcz, E.Dumiszewska, E.Dąbrowska, P.P. Michałowski, Ultramicroscopy 204 (2019) 6-9.

[6] I. Jóźwik, J. Jagielski, E. Dumiszewska, M. Kamiński, U. Kentsch, Ultramicroscopy 228 (2021) 113333.

Modeling of the behaviour of materials under irradiation

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

Abstracts of the posters
(Wednesday, November 17, session 1)

Modeling of the behaviour of materials under irradiation

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

Modeling of the behaviour of materials under irradiation

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

Evaluation of alternative oxides as a strengthening particles for ODS Reduced Activation Ferritic steels

Malgorzata FRELEK-KOZAK[1], Łukasz KURPASKA[1], Katarzyna MULEWSKA[1], Iwona JÓŹWIK[1,2], Maciej ZIELIŃSKI[1], W. Chmurzyński[1], Witold CHROMIŃSKI[3], Agata ZABOROWSKA[1], K. Kaszica[2], Jacek JAGIELSKI[1,2], Agata STROJNY-NĘDZA[2], Michał CHMIELEWSKI[2]

[1]NOMATEN Centre of Excellence, National Centre for Nuclear Research, A. Soltana 7 St., 05-400 Otwock, Poland. [2]Łukasiewicz Research Network – Institute of Microelecotronic and Fotonics, Wólczyńska 133 St., 01-919 Warsaw, Poland. [3]Warsaw University of Technology, Plac Politechniki 1 St., 00-661 Warsaw, Poland

Abstract

Oxide Dispersed Strengthened (ODS) steels are considered as next generation materials. They exhibit unique set of properties such as: outstanding mechanical parameters, chemical resistance, good weldability and high swelling resistance under heavy radiation [1]. The main objective of this research is to verify the alternative composition of ODS as material subjected to work under severe radiation damage. Commonly used Y2O3 is replaced with alternative oxides (Al2O3 or ZrO2) in a chromium reached steel. Both of selected compounds are characterized by sufficient thermal stability at the desired operating temperatures [2], thus they can be regarded as promising candidates for next generation ODS steels.

A steel powder with chemical composition of 12%wt.Cr, 2% wt. W, 0.3% wt. Ti and strengthening oxide of 0.3% Al2O3 or ZrO2 was first mixed in Ar-purged glove box and mechanically alloyed in the high energy planetary ball mill. In the next step, powder was consolidated by Spark Plasma Sintering technique. This procedure allowed to obtain bulk materials with high density (96-97% of the theoretical value of the steel). As a next step, specimens were subjected to ion irradiation Ar+ up to fluence 1x1016 ions/cm2 to introduce into the structure radiation defects. Structural and mechanical properties of manufactured ODS steel have been determined implementing the SEM/EBSD technique, X-ray diffraction analysis, microhardness and nanoindentation tests. Results were compared to properties of 12% Cr ODS steel strengthened with yttria (Y2O3). Obtained results have revealed a strong correlation between the type of strengthening oxide and mechanical properties as well as radiation resistance.

References

[1] C. Heintze et al., J. Nucl. Mater. 428 (2012) 139–146.

[2] J. Hoffmann et al., J. Nucl. Mater. 442 (2013) 444–448.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

The influence of manufacturing parameters on microstructure and mechanical properties of CoCrFeNi high entropy alloys produced via Mechanical Alloying and Spark Plasma Sintering

Artur OLEJARZ, Małgorzata FRELEK-KOZAK, Anna KOSIŃSKA, Iwona JÓŹWIK, Maciej ZIELIŃSKI, Marcin CHMIELEWSKI, Łukasz KURPASKA

NOMATEN Centre of Excellence, National Center for Nuclear Research, A. Soltana 7, 05-400 Otwock-Swierk, Poland

Abstract
During the last 15 years High Entropy Alloys (HEA) gained popularity within the scientific environment due to their promising performance in a wide temperature range [1]. Since the properties of HEA results from the chemical composition, the attention of researchers is focused on different compositions. Many of them have been evaluated experimentally presenting a beneficial combination of high strength, corrosion and fatigue resistance [2]. However, besides chemical composition, the chosen manufacturing method may also impact functional properties of high entropy alloys [3].

This preliminary work focuses on the CoCrFeNi HEA composition. The first step of this study concentrated on evaluating a wide spectrum of manufacturing parameters of the mechanical alloying process and choosing spark plasma sintering (SPS) conditions in reference to obtained microstructure and mechanical properties. Powders were mixed in Ar-purged glove box and milled in planetary ball mill with different milling time and rotation speed. Then, XRD, SEM and HV investigations were done in order to determine functional properties depending on synthesis parameters. Obtained preliminary results suggest, that mixing conditions severely impact obtained mechanical and structural properties of the studied system. Chemical composition of the matrix is rather uniform, but a lot of rich in Cr precipitates (with different sizes) have been detected.

References
[1] F. Otto, A. Dlouhý, C. Somsen, H. Bei, G. Eggeler, E.P. George, The influences of temperature and microstructure on the tensile properties of a CoCrFeMnNi high-entropy alloy, Acta Mater. 61 (2013) 5743.
[2] M. Li, Y. Guo, H. Wang, J. Shan, Y. Chang, Microstructures and mechanical properties of oxide dispersion strengthened CoCrFeNi high-entropy alloy produced by mechanical alloying and spark plasma sintering, Intermetallics. 123 (2020) 106819.
[3] F. Průša, A. Šenková, V. Kučera, J. Čapek, D. Vojtěch, Properties of a high-strength ultrafine-grained CoCrFeNiMn high-entropy alloy prepared by short-term mechanical alloying and spark plasma sintering, Mater. Sci. Eng. A. 734 (2018) 341.

Modeling of the behaviour of materials under irradiation

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

Experimental and computational study of intrinsic mechanical properties of pristine and irradiated Fe

Katarzyna MULEWSKA[a,b], Łukasz KURPASKA[a,b,c], Francisco Javier DOMÍGUEZ-GUTIÉRREZ[c], Iwona JÓŹWIK[b,e], Anna KOSIŃSKA[a], Witold CHROMIŃSKI[b,d], Jacek JAGIELSKI[a,c,e], Mikko ALAVA[a,b,f]

[a] NOMATEN Centre of Excellence, National Center for Nuclear Research, A. Soltana 7, 05-400 Otwock-Swierk, Poland. [b] National Center for Nuclear Research, NOMATEN MAB+ Division, A. Sołtana 7, 05-400 Świerk-Otwock, Poland. [c] NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Świerk/Otwock, Poland. [d] Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland. [e] Łukasiewicz Research Network – Institute of Microelecotronic and Fotonics, Wólczyńska 133 St., 01-919 Warsaw, Poland. [f] Department of Applied Physics, Aalto University, P.O. Box 11000, 00076 Aalto, Espoo, Finland

Abstract

Ferritic/martensitic steels are considered as materials for structural components of future generation fission and fusion reactors because the possess several promising properties like mechanical strength, corrosion and radiation damage resistance [1]. In order to better understand the behavior of these steels under extreme operating conditions, we carry out a combined experimental and numerical modelling study of the nanoindentation test. Experiments are conducted on pristine and irradiated iron, purity of 99.999%. Goal of our work is to investigate the transition between elastic to plastic deformation by analyzing pop-ins phenomenon in the load-displacement and strain-stress curves [2-4]. Scanning and transmission electron microscopes are used to investigate structural properties of the specimens. Spherical indenter tip is utilized to perform mechanical analysis. MD simulations and experimental results reached qualitative good agreements as shown in Fig 1-2. Our study aims to shed a light on the understanding of hardening of BCC metals and elastic–plastic contact points.

References

[1] S. Zinkle and J. Busby. Materials Today 12, 12 (2009).
[2] F. Pöhl, Scientific reports 9, 15350 (2019).
[3] M. A. Loades et al. Acta Materialia, vol. 59,pp. 4264–4273 (2011).
[4] S. Pathak and S. R. Kalidindi. Materials Science and Eng. R 91, 1-36 (2015).

Modeling of the behaviour of materials under irradiation

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

Understanding oxidation of zirconium and its alloys in air and water vapour operating conditions

Kinga SUCHORAB, Łukasz KURPASKA

NOMATEN Centre of Excellence, National Center for Nuclear Research, A. Soltana 7, 05-400 Otwock-Swierk, Poland

Abstract

Zirconium alloys are used for fuel cladding in nuclear reactors, where they act as a barrier separating the fuel from the coolant [2]. During operation, a cyclic corrosion process takes place. With each stage of the cycle, oxide phases and its physicochemical properties change [2-3]. In previous studies [1-3] it was reported that the corrosion kinetics depends on the chemical composition of alloys and various stabilization mechanisms of the tetragonal zirconium phase (t-ZrO_2). In this work, we present an experimental study of the oxidation kinetics of three zirconium-based materials. The oxidized samples were examined by Raman spectroscopy to obtain the phase distribution in the oxide and the percent content of the tetragonal phase depending on the distance from the metal/oxide interface. The obtained results are in perfect agreement with the previous studies [1,3] and additionally they shed new light on band shifts changes. These variables can be correlated with the compressive stress in a sample, which is one of the most important factors responsible for the stability of the tetragonal phase. In the future, experiments will be carried out under high steam temperature conditions, and samples will be irradiated with Cr, Zr, Ti or V. According to the theoretical research carried out by Youssef et al. [4] these are thermodynamic admixtures that minimize the solubility of hydrogen in zirconium oxide.

References

[1] C.M. Efaw, J.L. Vandegrift, M. Reynolds, B.J. Jaques, H. Hu, H. Xiong, M.F. Hurley, Characterization of zirconium oxides part II: New insights on the growth of zirconia revealed through complementary high-resolution mapping techniques, Corrosion Science 167 (2020) 108491 .

[2] A.T. Motta, A. Couet, R.J. Comstock, Corrosion of Zirconium Alloys Used for Nuclear Fuel Cladding, Annual Review of Materials Research 45 (2015) 311-343.

[3] J. Liu, H. Yu, P. Karamched, J. Hu, G. He, D. Goran, G. Hughes, A. Wilkinson, S. Lozano-Perez, C. Grovenor, Mechanism of the α-Zr to hexagonal-ZrO transformation and its impact on the corrosion performance of nuclear Zr alloys, Acta Materialia 179 (2019) 328-341.

[4] M. Youssef, M. Yang, B. Yildiz, Doping in the Valley of Hydrogen Solubility: A Route to Designing Hydrogen-Resistant Zirconium Alloys, Physical Review Applied 5 (2016) 014008.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Transmission Electron Microscopy as a tool for studying defects of irradiated materials

Witold CHROMIŃSKI

NOMATEN Centre of Excellence, National Centre for Nuclear Research, A. Soltana 7 St., 05-400 Otwock, Poland. Warsaw University of Technology, Faculty o Materials Science and Engineering, Wołoska 141, 02-507 Warsaw, Poland

Abstract

Transmission electron microscopy (TEM) allows to investigate structural defects like dislocations, grain boundaries, second phase precipitation or inclusions as well as nano voids created for example by helium irradiation. Most of the experiments in TEM are closely related to crystallographic alignment of defects since the sample act as a diffraction grid for incoming electrons [1]. For this reason, TEM studies can give detailed insight into the crystallographic nature of defects [2]. Besides some difficulties in performing experiments, TEM is considered as a very powerful tool which can provide detailed information about structural features unable to obtain with any other tool [3]. TEM data is mandatory if one wants to understand the nature of material deformation and impact of radiation damage on the mechanism of hardening. At NOMATEN we plan to study a variety of materials considered to be used in the next generation nuclear reactors.

Since the installation of the SEM/FIB system earlier this year, as well as a broad ion milling device, NOMATEN CoE gained access to proper equipment for performing structural analysis of almost all types of materials. FIB sections allows to prepare thin foils suitable for TEM investigations of the irradiated surfaces and regions below the indent which allows to link results obtained by the modeling group with microstructural and mechanical investigations. This poster is intended to present early results and capabilities of electron microscopy techniques available at NOMATEN CoE.

References

[1] M.L. Jenkins, Characterization of radiation damage by transmission electron microscopy, CRC Press 2000.

[2] W. Chrominski et al, TEM investigation of the influence of dose rate on radiation damage and deuterium retention in tungsten, Mater. Charact. 154 (2019) 1–6.

[3] W. Chrominski et al, Microstructure evolution in helium implanted self-irradiated tungsten annealed at 1700 K studied by TEM, Mater. Charact. 174 (2021) 110991.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

NOMATEN's XRAYLAB – The Newly-Created X-Ray Diffraction Laboratory

Maciej ZIELIŃSKI

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. Andrzeja Soltana 7, 05-400 Otwock, Poland

Abstract
At the beginning of May 2021 the Bruker D8 Advance all-purpose powder/polycrystalline X-Ray diffractometer has been installed in Department NOMATEN and operation of XRAYLAB – X-Ray Diffraction Laboratory has been launched. The 3 most valuable components of the diffractometer are:

- two Anton-Paar high-temperature *in-operando* chambers capable of reaching 1200°C with the environmental heating or up to 2000°C with the strip heater;
- the LYNXEYE XE-T strip detector covering the Cr up to Mo radiation and featuring brilliant energy resolution making K_β radiation filters redundant;
- Göbel mirror transforming the divergent Cu X-Ray beam produced typically by the sealed X-Ray tube into the parallel beam that opens wide range of applications.

Both the divergent and parallel beam are suitable for measurements aiming at phase identification and quantification as well as structure analysis (including: lattice parameters determination, crystals' size and shape assessment or even rough description of residual stress and, occasionally, structure solution) [1]. The parallel beam improves the capabilities of the diffractometer so that the following is possible: investigation of irregularly-shaped samples; depth-dependent analysis of thin coatings with grazing angle of incidence of the primary beam; reflectometry measurements for thin film thickness and roughness assessment; microdiffraction studies and mapping of specimen surface; investigation of residual stress in iso- and side-inclination modes; specimen texture determination. The Laboratory has already screened such materials as: Al_2O_3 anti-corrosion coatings on stainless steels; ODS steels; HEAs and thin films of HEA on Si wafers. The collaboration partnerships allow to simulate and model the structure of the investigated material including, among others, structure defects or quasicrystal ordering of scattering centres.

References
[1] B. E. Warren, X-Ray Diffraction, Addison-Wesley Publishing Company Inc., 1969.

Modeling of the behaviour of materials under irradiation

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

Annealing-induced strengthening in the NiCoCr alloy: The role of segregation

Axel POISVERT, A. NAGHDI, Kamran KARIMI, Amin ESFANDIARPOUR, Rene A. ALVAREZ DONADO, Pawel SOBKOWICZ, Mikko ALAVA, Stefanos PAPANIKOLAOU

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland

Abstract

Recent experiments by Ritchie et al. [1] and atomistic simulations by Ma et al. [2] have analyzed local ordering features associated with equiatomic medium entropy NiCoCr alloys and their dependence on additional thermal treatments such as annealing and aging processes. The experiments report on the emergence of short-range (structural) ordering in aged samples with strong impacts on mechanical properties (i.e. dislocation activation energy and hardness). The numerical work interprets the growth of annealing-induced Ni-based nano-precipitates as the main source of structural heterogeneities leading to significant work hardening at bulk scales. This has been evidenced by a pronounced reduction of the stacking fault width upon shearing which tends to show strong correlations with the annealed samples' strengthening. Here, we performed hybrid Monte Carlo-Molecular Dynamics simulations based on two well known NiCoCr interatomic potentials. As reported in [3], we find that the emergence of segregated (Ni-based) phases upon annealing is not a robust feature but may also depend on the chosen energy potential. Following the numerical framework in [2], we probed effects of the annealing process in terms of atomistic pressure fluctuations, stacking fault widths (including edge and screw dislocations), as well as the specific heat and thermal expansion coefficient. In particular, our analysis indicates meaningful variations of dislocation separation widths with the concentration of local (chemical) ordering, distinguishing the annealed samples from single-phase mixed solid solutions. Whether or not the observed correlations lead to an effective strengthening mechanism has yet to be established.

References

[1] Zhang, Ruopeng, Shiteng Zhao, Jun Ding, Yan Chong, Tao Jia, Colin Ophus, Mark Asta, Robert O. Ritchie, and Andrew M. Minor. "Short-range order and its impact on the CrCoNi medium-entropy alloy." *Nature* 581, no. 7808 (2020): 283-287.

[2] Li, Qing-Jie, Howard Sheng, and Evan Ma. "Strengthening in multi-principal element alloys with local-chemical-order roughened dislocation pathways." *Nature communications* 10, no. 1 (2019): 1-11.

[3] A. Naghdi, A. Poisvert, K. Karimi, A. Esfandiarpour, R. Alvarez, P. Sobkowicz, M. Alava, S. Papanikolaou, Nanoprecipitates, defects and strengthening in concentrated solid solutions: The intriguing case of NiCoCr, in preparation, 2021.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Molecular dynamics simulation of interface structure and shape of Nb precipitate in Zr matrix

Zhengxuan FAN, Emmanuel CLOUET

Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette, France

Abstract

Zr-Nb alloys containing 1-2.5% Nb are successfully used for the fuel cladding in nuclear power plants because of their good mechanical properties and good in-reactor corrosion resistance. Under neutron irradiation, body-centered-cubic β-Nb nano-precipitates develop within the hexagonal-close-packed α-Zr matrix [1]. In this work, we carried out molecular dynamics simulations to study these Nb precipitates in the Zr matrix. An EAM potential has been developed for this purpose, which gives a good description of the alloy, such as its basic physical properties, solution energies, and solute binding energies.

Planar Zr-Nb interfaces are first studied, with Pitsch -Schrader orientations between the precipitate and the matrix as observed experimentally. The interface structures which gives lowest energies are identified. The excess energies of these interfaces are compared to the values obtained from ab initio calculations, as well as with other empirical inter-atomic potentials. Simulations of 3D precipitates are then carried out to find the shape of the precipitate that minimizes its formation energy, for both coherent and semi-coherent interfaces containing misfit dislocations. It is found that misfit dislocations effectively decrease precipitate formation energy. The optimal number of dislocations at the interfaces is the one which cancels the lattice misfit between the β-Nb precipitates and the α-Zr matrix in order to reduce the elastic energy stored in the precipitate. Elastic energy appears thus dominant in the control of precipitate formation energy, compared to the cost of interfaces. Precipitates with semi-coherent interfaces have a platelet shape elongated in the basal plane which is quite similar to that observed experimentally [1].

References

[1] J. Ribis, S. Doriot, and F. Onimus, Shape, orientation relationships and interface structure of beta-Nb nano-particles in neutron irradiated zirconium alloy, J. Nucl. Mater. 511, 18–29 (2018).

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Thermodynamic modeling of Ti-O from ab initio calculations

Martin-Stéphane TALLA NOUTACK, Emmanuel CLOUET

Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette, France

Abstract

It has been recently evidenced from transmission electronic microscopy [1] the capability of the oxygen atoms to order in titanium alloys even for low oxygen content. These ordered structures correspond to the Ti6O-type precipitates having the same crystalline structure as the matrix (namely α-hcp lattice) but with the oxygen atoms ordered in the interstitial sites instead of being randomly distributed. In addition, atom probe tomography (APT) as well as small-angle X-ray scattering (SAXS) analyses show that these ordered domains display an almost similar composition as the matrix. In other words, no local variation of the chemical composition is noticed. X-ray diffraction experiments also point out a slight increase in the lattice parameters [1] related to these ordered precipitates. The objectives of this work is thus i) to study the possibility to form ordered compounds having a Ti6O-type structure with no chemical partitioning of oxygen and, ii) to investigate whether this ordering would be associated to an increase of the lattice parameters. Our work shows, by evaluating the formation enthalpies of different ordered and disordered compounds in the Ti - Ti6O composition range, that, for a given composition, the ordered structures are always more stable than disordered ones, in agreement with experiments [1]. However, no intermediate stable structure is found below the convex hull linking Ti and Ti6O. According to thermodynamics, a supersaturated Ti-O solid solution should decompose in Ti and Ti6O phases, contrary to experiments that evidence intermediate stable ordered compounds. In order to understand the origin of this discrepancy, we envisage studying kinetics of decomposition and ordering in Ti-O. For this, we build an energetic model from our DFT data aiming at describing the effective interactions between oxygen atoms. We show that an Ising model only based on pair interactions is sufficient to describe oxygen-oxygen effective interactions. Kinetic Mote Carlo simulations using this rigid lattice energy model will be further developed to study the kinetic evolution of Ti-O supersaturated solid solutions. Furthermore, we show in agreement whit experiments [2] that the lattice parameters increase with oxygen content and that this increase is more important for c than for a parameter. However, no difference is observed between ordered and disordered structures unlike what is pointed out in experiments. It appears necessary, in a second step, to go beyond 0 K calculations by considering the contribution of the vibrational free energy within the quasi-harmonic approximation.

References

[1] Poulain et al. “Oxygen ordering in titanium alloys achieving a unique combination of strength and ductility”, submitted (2021).

[2] Wiedemann et al. “Microhardness and lattice parameter calibrations of the oxygen solid solutions of unalloyed -titanium and Ti-6Al-2Sn-4Zr-2Mo”, Metall. Trans. **18,** 1503-1510 (1987).

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Potential oxygen scavenger chemicals for secondary side chemistry cycles

Konsta SIPILÄ

VTT Technical Research Centre of Finland, P.O. Box 1000, FI-02044 VTT, Finland

Abstract

Hydrazine is an excellent oxygen scavenger and passivation promoter used in nuclear power plants routinely. Hydrazine influences corrosion by three separate ways. As hydrazine possesses potential health and environmental hazards, it is possible that its use will be banned. Therefore, a search for substitutes is needed and a comprehensive experimental campaing to study proper alternatives has been performed by VTT. This campaing includes four candidate chemicals (erythrobic acid (EA), carbohydrazide (CH), diethyl-hydroxylamine (DEHA) and methyl-ethyl-ketoxime (MEKO)). Their oxygen scavenging efficiency was experimentally compared at room temperature [1], in a simulated SG revision period environment (T = 50°C) [2] and at high temperature (T=228°C) [3]. Electrochemical measurements and commercially available oxygen sensors were applied in the scavenging efficiency measurements. Based on the results, EA and CH seem to have a similar scavenging efficiency as hydrazine. Measurement results with MEKO and DEHA indicated poorer scavenging ability and in case of MEKO, unique decomposition kinetics was observed (most probably due to the formation of N2O) that interfered oxygen level measurements with the commercial oxygen sensor.

References

[1] Betova, I., Bojinov, M. and Saario, T. 2017. Kinetics of oxygen removal by hydrazine alternatives in condi-tions of steam generator preservation during outage. VTT Research Report VTT-R-05209-17.
[2] Betova, I., Bojinov, M. and Saario, T. 2018. Hydrazine alternatives as oxygen scavengers and passivation agents in steam generator preservation conditions. VTT Research Report VTT-R-01908-18.
[3] Essi Jäppinen, Tiina Ikäläinen, Frej Lindfors, Timo Saario, Konsta Sipilä, Iva Betova, Martin Bojinov. A comparative study of hydrazine alternatives in simulated steam generator conditions—Oxygen reaction kinetics and interaction with carbon steel, Electrochimica Acta, Volume 369, 2021, 137697, ISSN 0013-4686, https://doi.org/10.1016/j.electacta.2020.137697.

Modeling of the behaviour of materials under irradiation

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

Abstracts of the posters
(Thursday, November 18, session 2)

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Structure-based optimization of crystal plasticity parameters in metal alloys

Karol FRYDRYCH, Stefanos PAPANIKOLAOU

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland

Abstract
In order to model behaviour of materials in the plastic regime, it is critical to identify precise model parameters. Commonly, such selection is either performed using trial and error approaches or fitting algorithms. Here, we focus on evolutionary algorithms (EA) that may also perform such an optimization. The objective is to minimize the difference between simulated and experimentally measured load-deformation (stress-strain) curves. We show how such an approach was applied to optimize crystal plasticity parameters using the viscoplastic [1] and elasto-viscoplastic [2] self-consistent models in Mg alloy sheets and Cu films, under multiaxial loading conditions. Such an optimization may be augmented by using structure-based information, such as differences between crystallographic textures [3]. We will show prior applications of such approaches and our recent progress on the possibility to optimize the parameters based on matching surface deformation data obtained in nanoindentation tests. Such an approach is very important, especially in the case of ion-implanted materials where nanonindentation is often the only way to examine material properties due to the small thickness of the irradiated layer.

References
[1] Frydrych K., Libura T., Kowalewski Z., Maj M., Kowalczyk-Gajewska K., On the role of slip, twinning and detwinning in magnesium alloy AZ31B sheet, Materials Science and Engineering A, Vol.813, pp.141151-1-14, 2021.
[2] Girard G., Frydrych K., Kowalczyk-Gajewska K., Martiny M., Mercier S., Cyclic response of electrodeposited copper films. Experiments and elastic-viscoplastic mean-field modeling, Mechanics of Materials, Vol.153, pp.103685-1-103685-17, 2021.
[3] Frydrych K., Jarzębska A., Virupakshi S., Kowalczyk-Gajewska K., Bieda M., Chulist R., Skorupska M., Schell N., Sztwiernia K., Texture-based optimization of crystal plasticity parameters: application to zinc and its alloy, Metallurgical and Materials Transactions A, Vol.52, No.8, pp.3257-3273, 2021.
[4] Frydrych, K.; Karimi, K.; Pecelerowicz, M.; Alvarez, R.; Dominguez-Gutiérrez, F.J.; Rovaris, F.; Papanikolaou, S. Materials Informatics for Mechanical Deformation: A Review of Applications and Challenges. Preprints 2021, 2021090176 (doi: 10.20944/preprints202109.0176.v1).

Modeling of the behaviour of materials under irradiation

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

Shear banding instability in high entropy multi-component metallic glasses: The role of composition and order

Kamra KARIMI, Amin ESFANDIARPOUR, Rene Alberto ALVAREZ DONADO, Mikko ALAVA, Stefanos PAPANIKOLAOU

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland

Abstract

The shear band instability in quasi-statically driven bulk metallic glasses (BMGs) emerges from collective dynamics mediated by shear transformation zones (STZs). It is phenomenologically known that sharp structural features of shear bands are correlated to the sharpness of the plastic yielding transition, being very high in the commonly studied limit of alloys with very different elements in terms of their atomic radii. However, in the opposite limit of high-entropy multicomponent alloys (with similar atomic radii), yielding of a BMG is highly dependent on compositional/ordering features. Here, we report on simulations of multi-component BMG with different elements showing that the interplay between composition-driven icosahedra-ordering and collectively-driven STZs controls the degree of strain localization [1]. We quantify yielding by measuring the atoms' susceptibility to rearrangements that correlates to the structure. We find that the abundance of icosahedral clusters increases BMG's capacity to delocalize strain. The plastic yielding can be inferred by one of the commonly used compositional descriptors that characterize element associations, the misfit parameter δ_α, or by shear-band width and correlation parameters. The predictability of bulk response based on elemental and microstructural features paves the way for applications of machine learning within the structure-property paradigm [2,3].

References

[1] Karimi, K., Esfandiarpour, A., Alvarez-Donado, R., Alava, M., Papanikolaou, S., Shear banding instability in high entropy multi-component metallic glasses: The role of composition and order, in preparation.

[2] Frydrych, K., Karimi, K., Pecelerowicz, M., Alvarez, R., Dominguez-Gutiérrez, F. J., Rovaris, F., & Papanikolaou, S. (2021). Materials Informatics for Mechanical Deformation: A Review of Applications and Challenges, submitted to MDPI.

[3] Jeon, J., Seo, N., Kim, H. J., Lee, M. H., Lim, H. K., Son, S. B., & Lee, S. J. (2021). Inverse Design of Fe-Based Bulk Metallic Glasses Using Machine Learning. Metals, 11(5), 729.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Features of solid solution hardening in face-centered cubic random high entropy alloys: MD simulation

Amin ESFANDIARPOUR, Stefanos PAPANIKOLAOU, Mikko ALAVA

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland

Abstract

High entropy alloys (HEAs) have attracted much attention within the materials science community owing to an ever-increasing demand for their potential application as structural components in nuclear reactors with superior mechanical properties. One of the sources of excellent mechanical properties of HEAs is unconventional dislocation responses to applying stresses, in comparison to traditional alloys. In this study, we investigated the edge dislocation geometry and its mobility under applying stress in several face-centered cubic (FCC) single-phase solid solution alloys (i.e., CrCoNi, CrMnCoNi, CrFeCoNi, CrMnFeCoNi, FeNi, and also, Fe0.4Mn0.27Ni0.26Co0.05Cr0.02, Fe0.7Ni0.11Cr0.19) using molecular dynamics. Correlation length, saturation roughness, and stacking fault width as a function of applying stress are presented in this study. According to our findings, close to depinning stress (σc), all these parameters were maximum. The velocity of dislocations, as a function of applying stress, was calculated for these alloys. Our results showed that dislocation in the stronger alloys (i.e., CrCoNi, CrMnCoNi, CrFeCoNi, and CrMnFeCoNi) moves slower than the traditional alloys. The top four stronger alloys demonstrated overhang in the two partial dislocation lines. Yield stress from the analytical model was compared with depinning stress and the results were discussed. The ratio of saturation roughness to stacking fault width at depinning stress rescaled with σc. This suggests that for single phase solid solution alloys, one of the strategies to increase strength is the combined design of stacking fault width and element-based chemical disorder.

References

[1] Tsai M H and Yeh J W 2014 Materials Research Letters 2 107– 123.
[2] Levo E, Granberg F, Utt D, Albe K, Nordlund K and Djurabekova F 2019 Journal of Materials Research 34 854–866.

Modeling of the behaviour of materials under irradiation

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

Configurational entropy in High entropy metallic glasses

Rene Alberto ALVAREZ DONADO, Amir ESFANDIARPOUR, Stefanos PAPANIKOLAOU, Mikko ALAVA

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland

Abstract

We determine the behaviour of the configurational entropy for a set of multi-principal element alloys in their crystalline and vitreous states numerically. Our results show that the ideal mixing entropy formula Smix=− ∑ Xi(logXi)does not only overestimates, but it is incapable of providing any structural or thermodynamic information about the formation mechanism of the multi-element alloys. We employ Molecular dynamics and swapping Monte Carlo simulations in combination with the reversible scaling method to efficiently compute the real configurational entropy, and to shed light on how its value relates to obtaining solid solutions when annealing at different temperatures or glasses if the vitreous transition is favourable. These results will prepare the way for determining single solid solution high entropy alloy as well as high entropy metallic glasses.

References

[1] S. Sastry, Nature409, 164 (2001).
[2] L. Berthier and G. Biroli, Rev. Mod. Phys.83, 587(2011).
[3] M. Ozawa, C. Scalliet, A. Ninarello, and L. Berthier, J.Chem. Phys.151, 084504 (2019).
[4] R. Paula Leite, R. Freitas, R. Azevedo, and M. de Kon-ing, J Chem. Phys.145, 194101 (2016).
[5] R. Freitas, M. Asta, and M. de Koning, Comput. Mater.Sci.112, 333 (2016).

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Discrete Dislocation Dynamics Simulations with Free Surfaces: Applicaton to Mechanical Testing of Micropillars

Fabrizio ROVARIS, Stefanos PAPANIKOLAOU, Mikko ALAVA

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland

Abstract
We present a Discrete Dislocation Dynamics (DDD) approach able to handle the problem of free surfaces [1]. The DDD code is coupled to a Finite Element solver following the Discrete Continuous Model [2] to allow for the exact numerical treatment of the stress fields in the presence of generic free surface geometries.
Our DDD approach is then used to simulate the micromecanical testing of micropillars, particularly investigating the effect of a small curvature on the top free surface of the pillars. This is directly compared with the results obtained for the uniaxial testing of standard, flat pillars. The results for the compression of flat micropillars show a homogeneous stress field inside the pillar and dislocation sources randomly activated inside the volume, as expeteced during uniaxial testing. On the other hand, the presence of an even small curvature on top of the micropillars leads to a completely different evolution of the dislocation microstructure, with an overestimation of the strain at yielding due to an incorrect evaluation of the elastic regime in the stress/strain curve.

References
[1] F. Rovaris et al., in preparation (2021).
[2] O. Jamond et al., International Journal of Plasicity 80, 19-37 (2016).

Modeling of the behaviour of materials under irradiation

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

Structural, mechanical and electrical properties of ion-irradiated polymers used as cable insulation

Anna KOSIŃSKA[1)], Jacek JAGIELSKI[1,2)], Iwona JÓŹWIK[2,3)], Magdalena WILCZOPOLSKA[1)], D. BIELIŃSKI[4)], Michał OKRASKA[4)], Edyta WYSZKOWSKA[1)], Mélanie CLOZEL[1)]

[1)] National Centre for Nuclear Research, 7th A. Soltana Str., Świerk-Otwock, Poland. [2)] Lukasiewicz Research Network - Institute of Microelectronics and Photonics, Al. Lotników 32/46, Warsaw, Poland. [3)] NOMATEN CoE, NOMATEN MAB, National Centre for Nuclear Research, Department of Physics, 7th A. Soltana Str., Świerk-Otwock, Poland. [4)] Institute of Polymer and Dye Technology, Lodz University of Technology, Stefanowskiego 12/16, 90-924 Lodz, Poland

Abstract

Electrical cables and wires are an integral part of a nuclear power plant (NPP) instrumentation, control and security systems [1]. Cables are continuously vulnerable to variety of environmental stressors like high temperature, gamma radiation, humidity, chemicals and mechanical stresses. It is known that the structure of polymer materials changes under the influence of radiation and the alterations like chains scission and cross-linking occur [2-3]. These phenomena determine the lifetime of the cables. Main structural effect caused by heavy ions is a massive loss of hydrogen from the surface layer which leads to its smoothening, shrinkage and loss of resistivity [4-5]. Ion irradiation of polymeric materials changes their chemical and physical properties similarly to the gamma radiation. Non-elastic interactions of ions with electrons are a good analogue to the impact of gamma radiation. The aim of the recent works was to investigate the correlation between hardness and resistance of different type of polymer insulation. In this study, the structural properties of pristine and irradiated polymer insulation were assessed by means of Scanning Electron Microscopy. The phase composition was identified by Raman spectroscopy technique. The functional properties were obtained by using nanoindentation method, wear tests and electrical measurement. The results show that the electrical resistance decreases, while there is an increase in hardness with increasing ion irradiation fluence.

References

[1] Nuclear Power Reactors in the World IAEA, Vienna (2020).
[2] R.L. Clough, Nucl. Instr. and Meth. B 185 (2001).
[3] T. Seguchi, K. Tamura, T. Ohshima, A. Shimada, H. Kudoh, Radiation Phys. Chem. 80 (2011).
[4] A. Kosińska, J. Jagielski, Ł. Kurpaska, E. Wyszkowska, M. Clozel, J. Zagórski, B. Staszkiewicz, K. Gniadek, Nucl. Instrum. Methods B (2020).
[5] A. Kosińska, J. Jagielski, M. Wilczopolska, D.M. Bieliński, M. Okraska, I. Jóźwik, Ł. Kurpaska, K. Nowakowska-Langier, Surf. Coat. Technol. (2020).

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Synthesis of high-entropy alloy coatings obtained by magnetron sputtering

Magdalena WILCZOPOLSKA[1], Katarzyna NOWAKOWSKA-LANGIER[1], Grzegorz STRZELECKI[1], Sebastian OKRASA[1], Anna KOSIŃSKA[1], Iwona JÓŹWIK[2,3], Maciej ZIELIŃSKI[1,3], Katarzyna MULEWSKA[1,3]

[1]National Centre for Nuclear Research, 05-400 Otwock, Poland. [2]Lukasiewicz Research Network - Institute of Microelectronics and Photonics, Al. Lotników 32/46, Warsaw, Poland. [3]NOMATEN CoE, NOMATEN MAB, National Centre for Nuclear Research, Department of Physics, 7th A. Soltana Str., Świerk-Otwock, Poland

Abstract
This work represents the initial stage of synthesis of multi-component alloys layers characterized by high entropy using magnetron sputtering methods. High entropy alloy layers are known due to the features they exhibit such as the effect of high entropy, lattice torsion, sluggish diffusion, and cocktail effect [e.g.1]. The method of magnetron sputtering used in this work
is a well-known frequently used method for the synthesis of materials in the form of layers.
The synthesis processes were carried out in a single-magnetron device by using pulse magnetron sputtering (PMS) [2] and gas injection magnetron sputtering (GIMS) [3] methods. The source of the components included in the layers were various multi-component (mosaic, sintered) targets.
Morphology and phase composition of the coatings were investigated by Scanning Electron Microscopy (SEM) and X-ray diffraction measurements. Mechanical properties were studied by means of nanoindentation technique. Preliminary studies have shown that plasma control using a sequence of electrical impulses (PMS) and periodically variable pressure (GIMS) results in an extremely favorable change in the structure and properties of layers, produced by the above-mentioned methods.

References
[1] Junchen L.; Yongxian H.; Xiangchen M.; Yuming X. A. Review on High Entropy Alloys Coatings: Fabrication Processes and Property Assessment. Advanced Engineering Materials 2019, 21(8):1900343, DOI: 10.1002/adem.201900343.
[2] Nowakowska-Langier K.; Chodun R., Minikayev R.; Okrasa S.; Strzelecki G.W., Wicher B.; Zdunek K. Copper nitride layers synthesized by pulsed magnetron sputtering. Thin Solid Films 2017, 645, DOI: 10.1016/j.tsf.2017.10.042.
[3] Zdunek K.; Nowakowska-Langier K.; Dora J.; Chodun R. Gas injection as a tool for plasma proces control during coating deposition. Surf. Coat. Technol.2013, 228(1) S367-S373, DOI: 10.1016/j.surfcoat.2012.05.101.

Modeling of the behaviour of materials under irradiation
November 16-19, 2021 (Société Géologique de France, 77 Rue Claude Bernard, 75005 Paris)

Challenges concerning industry partnerships and communication towards companies, science and public sector

Maciej DROZD, Maciej KOMOROWSKI

NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland

Abstract
At NOMATEN CoE, Industry Liaison Officer (ILO) and Communication and Dissemination Officer (CDO) cover two different areas in terms of official structure of the NOMATEN as well as in reference to the grant aggreement and other documents. ILO is
a member of the Industry Liaison Group that will hire more employees according to the needs and developed projects. CDO is a part of the Operation Office. Both experts report nowadays to the Director for Scientific Operations, however, in the future the new chief manager of the Operations Office will appear.
Nevertheless, the Industry Liaison Officer (ILO) and the Communication and Dissemination Officer (CDO) work in general together as a small task force focused on promoting NOMATEN among potential partners. Moreover, they are both engaged in the entire National Centre for Nuclear Research (NCBJ) communication and partnerships. Such group at NCBJ has been created by the Science and Technology Park at NCBJ and acts as a focal point for industrial partnerships as well as communication towards companies. Such activities will also cover potential team up between NCBJ, CEA and VTT towards the markets.
The poster presents challenges faced by the NOMATEN's team that consists of the Industry Liaison Officer (ILO) and the Communication and Dissemination Officer (CDO). Since promoting the portfolio of scientific achievements and services for industry requires different tools and abilities from regular sales and marketing background, the challenges are also not the same as in case of offering the deployment-ready products.

References
/

Modeling of the behaviour of materials under irradiation

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

Crystal plasticity law calibration of non-irradiated and proton irradiated 304L austenitic stainless steel

Rachma AZIHARI[1,2], Jérémy HURE[1], Marc LEGROS[2], Benoît Tanguy[1]

[1]Université Paris-Saclay, CEA, Service d'Etude des Matériaux Irradiés, 91191, Gif-sur-Yvette, France. [2]CEMES-CNRS, Toulouse, France

Abstract

Austenitic stainless steels are used in the nuclear industry to make the internals parts of Pressurized Water Reactors (PWR) such as baffles and former plates. Baffle-to-Former Bolts (BFB) experience Stress Corrosion Cracking under irradiation, which may lead to intergranular fracture. The fracture is induced by the Irradiation Assisted Stress Corrosion Cracking (IASCC) phenomenon. The understanding of this degradation mechanism is still incomplete due to complex interactions between irradiation-induced modifications of the microstructure and environmental effects. In order to predict the cracking of the grain boundary through a micro-mechanical approach, it is necessary to determine the intragranular mechanical behavior of the steel and the grain boundary strength.

Micro-pillars compression is used to yield experimental data on the mechanical behavior at the crystal scale. 500nm to 10µm diameter pillars are milled in non-irradiated and 1dpa proton irradiated 304L austenitic stainless steel using Focus Ion Beam after EBSD mapping to determine the crystal orientations. The pillars are tested at 10nm/s using a FT-NMT04 nanoindenter with a diamond flat punch at room temperature. The large range of the pillar diameters shows a size effect on the mechanical properties. Finite Elements numerical simulations of the micro-compression tests are set up using crystal plasticity constitutive equations developed for (non-)-irradiated austenitic steels [1]. A reverse optimization algorithm is used to match the experimental data and the simulations results, allowing accessing the behavior law parameters.

References

[1] X. Han, Modélisation de la fragilisation due au gonflement dans les aciers inoxydables austénitiques irradiés, PhD thesis, Mines ParisTech & CEA, 2012.

Modeling of the behaviour of materials under irradiation

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

Study of Ni based alloys obtained by Additive Manufacturing

Martin MADELAIN[1], Yann DECARLAN[1], Pascal AUBRY[2], Alexandre Legris[3]

[1]Université Paris-Saclay, CEA, Service de Recherches Métallurgiques Appliquées, 91191, Gif-sur-Yvette, France. [2]Université Paris-Saclay, CEA, Service d'Études Analytiques et de Téactivité des surfaces, 91191, Gif-sur-Yvette, France. [3]Polytech'Lille, UMET, Université Lille 1, France.

Abstract

Additive manufacturing offers new perspectives for complex parts with specific microstructures. Different challenges remain with this type of manufacturing. This work is part of the studies conducted on Molten Salt Reactord (MSRs) [1]. New material challenges emerge for this application, mainly the behavior under irradiation and corrosion from molten salts [2]. Many options remain in terms of design or choice of materials of structure. Addivite manufacturing is considered to design new parts, but this technique need to be evaluated for the materials of interest. Differents Ni based alloys are considered in this study. After a first manufacturing campaign, the objective is to find appropriate building parameters to obtain an healthy material. Different types of characterizations have been made to evaluate the density, hardness and microstructure of the alloys. With these characterizations, optimized parameters will be used to build other samples. Ion irradiation and corrosion studies will be carried to propose a first assesment of the behavior of this type of material in MSR environnment.

References

[1] Jérôme Serp, Michel Allibert, Ondřej Beneš, Sylvie Delpech, Olga Feynberg, Véronique Ghetta, Daniel Heuer, David Holcomb, Victor Ignatiev, Jan Leen Kloosterman, Lelio Luzzi, Elsa Merle-Lucotte, Jan Uhlíř, Ritsuo Yoshioka, Dai Zhimin, The molten salt reactor (MSR) in generation IV: Overview and perspectives,Progress in Nuclear Energy,Volume 77, 2014, Pages 308-319, ISSN 0149-1970.

[2] P. Yvon, F. Carré, Structural materials challenges for advanced reactor systems, Journal of Nuclear Materials, Volume 385, Issue 2, 2009, Pages 217-222, ISSN 0022-3115.

Modeling of the behaviour of materials under irradiation

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

Modeling of the behaviour of materials under irradiation

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

Selected visits (CEA Paris-Saclay)
(Friday, November 19)

Modeling of the behaviour of materials under irradiation

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

Modeling of the behaviour of materials under irradiation

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

LECI facility

The Laboratory for Studies on Irradiated Fuel (LECI) located on the Paris-Saclay site of the CEA, started operation in 1959. Nowadays the LECI facility is dedicated to the characterization of non-fissile materials, mostly metallic alloys, irradiated in MTR, LWR and SFR reactors. The main objectives are to determine the behavior of materials, like claddings, internals, pressure vessels, steam generator or primary circuit components, in normal, accidental, or (intermediate) storage conditions, and to predict the in-service lifetime of materials through the development of models. The installation is managed by a Service (SEMI, Section of Research on Irradiated Materials) through three R&D laboratories and one operating section (SEL) for operational support, maintenance and security and safety issues.

The LECI hot lab facility is composed of 3 lines with 45 shielded cells, where nuclearized equipments for machining, metallurgical, mechanical, and physico-chemical characterizations, are operated.

The LM2E laboratory is in charge of studying irradiation damages at a microscopic scale by means of optical microscopes, scanning (SEM) and transmission (TEM) electron microscopes, tomographic atomic probe (TAP), and a focused ion beam (FIB) equipment for preparing TEM and TAP samples. The laboratory is particularly skilled in metallographic preparations and observations, and also conducts studies on corrosion mechanisms and kinetics using specific corrosion loops and autoclaves.

The LPCMI laboratory carries out physico-chemical analyses and characterizations on irradiated materials among which gas sampling and analysis, density measurements, or determination of chemical composition by electron probe for microanalysis (EPMA). Moreover, the laboratory is in charge of machining of irradiated specimens with controlled geometries for further mechanical testing. Milling and turning machines, wire electrical discharge machines, or welding techniques are among the nuclearized machining equipments.

The LCMI laboratory is conducting research related to the mechanical properties using both mechanical tests and numerical simulation, in order to define damage and failure processes and set appropriate material behavior equations. Experimental studies are carried out with static and dynamic tensile tests, Charpy impact tests, toughness tests, axial creep and relaxation tests, pressurized tests on cladding tubes, and stress corrosion cracking tests. Inspection equipments and dimensional measurements complete the experimental capacities.

Through internal (CEA), national, european and international cooperations, technical and scientific approaches are continuously developed at the LECI to better address current and future issues related to the effect of irradiation on the properties and behavior of materials.

Shielded cells (line M) at the LECI hot laboratory (CEA Saclay, DES)

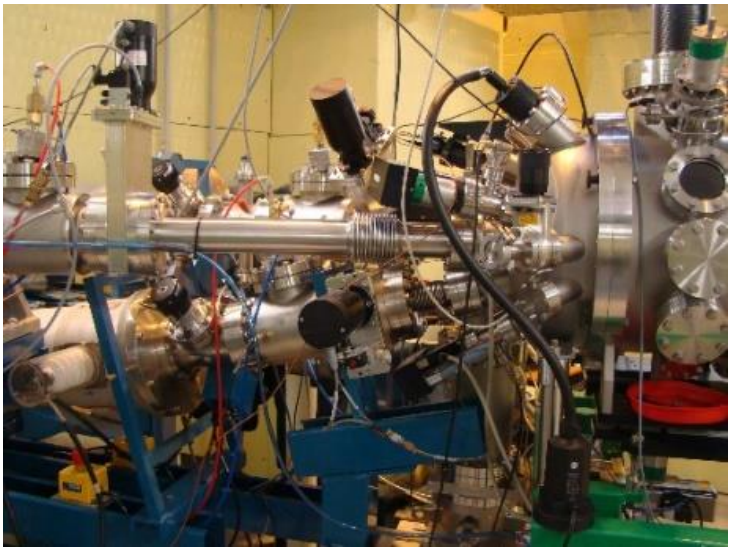
Modeling of the behaviour of materials under irradiation

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

JANNuS-Saclay triple ion beam facility

JANNuS-Saclay ion irradiation platform offers (DES/ISAS/DMN) the rare possibility to simultaneously deliver three concurrent ion beams on a single target allowing for a wide range of irradiation and implantation conditions for well-controlled modelling-oriented experiments. Ion beams are employed to understand neutron-induced effects in nuclear materials for decades as they can produce nuclear recoil damage and implant a large variety of elements mimicking helium and hydrogen from nuclear reactions, transmutation products, fission products and gasses. Among the most stringent reasons for using electrostatic ion accelerators are the scarcity of neutrons sources and the ease of use: a high damage level either as implanted ions and/or as dpa is obtained over a very short time – typically a few hours – and the irradiated sample has no residual radioactivity. Ion beams allow also to perform well controlled experiments in terms of energy, dose, flux, temperature. This is of great value in an analytical approach.

At CEA Paris-Saclay, a triple beam facility has been installed for simultaneous ballistic damage, gas implantation and/or electronic excitation. Samples can be irradiated in the wide temperature range from liquid nitrogen to 800°C. Evolution in the ion-irradiated material microstructure and changes in the service properties (mechanical, thermal…) are then characterized by on line Raman spectrometry or post mortem. Simulation can greatly help in validating the transposition of material laws derived from ion irradiations – formation and evolution of defect loops and of cavities, segregation, amorphization– to in-reactor conditions. The JANNuS-Saclay facility comprises three electrostatic accelerators (respectively named Épiméthée, Japet and Pandore) connected to a triple beam chamber for single-, dual- and triple beam irradiations. Three other chambers are linked to Épiméthée and Pandore for single beam irradiation and/or Ion Beam Analysis. The layout is divided into six linked rooms, separated by suitable concrete walls for radioprotection safety.



JANNuS-Saclay triple beam irradiation chamber (CEA Saclay, DES)

Modeling of the behaviour of materials under irradiation

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

Bioorganic Chemistry and Isotopic Labelling unit

The Bioorganic Chemistry and Isotopic Labelling (DRF/SCBM) is unit of the Frédéric Joliot Institute for Life Sciences, located in CEA Saclay which was established in 1965 with the mission of producing radiolabeled compounds for medical applications. While maintaining its expertise in radiolabeling (late stage isotopic labelling), the department has since initiated numerous research programs from basic research in bioorganic chemistry (medicinal chemistry, chemical biology) and nanosciences (drug delivery systems, catalysis) to its applications on biological systems. The visit will focus on three specific laboratories of the department, which are unique of their kind. Visits of this unit will include the following laboratories:

Tritium Isotopic Labeling Laboratory
This is a unique laboratory in Europe as regards its ability to radiolabel organic molecules with tritium, the radioactive isotope of hydrogen. The tritiation set-up uses tritium gas as the starting material, which is handled in a glove box and using a state-of-the-art manifold, allowing precise and safe control of the reaction parameters.

Radioactive Waste Remediation Laboratory
The facility consist of a low power inductive plasma generator that has been developed for the remediation of radioactive organic wastes by pyrolysis (Idhol). This set-up is an alternative to conventional incinerators that are not suited for corrosive and highly radioactive materials.

High Throughput Screening Laboratory
The robotic HTS platform is dedicated to the identification of small molecules modulating biological phenomena by a random screening approach. The approach consists in testing in parallel a library of molecules (up to 100 000) against a biological target, and studying the biological response to these molecules.

Frédéric Joliot Institute for Life Science, SCBM hot laboratories (CEA Saclay, DRF)

Modeling of the behaviour of materials under irradiation

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

Modeling of the behaviour of materials under irradiation

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

List of participants

Modeling of the behaviour of materials under irradiation

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

Modeling of the behaviour of materials under irradiation

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

List of participants (1/2)

Family Name	First Name	Company	Country	e.mail
ALAVA	Mikko	NCBJ (NOMATEN)	Poland	mikko.alava@ncbj.gov.pl
ALVAREZ DONADO	Rene Alberto	NCBJ (NOMATEN)	Poland	rene.alvarez@ncbj.gov.pl
ARFFMAN	Pentti	VTT	Finland	pentti.arffman@vtt.fi
AZIHARI	Rachma	CEA Saclay	France	rachma.azihari@cea.fr
BÉCHADE	Jean-Luc	CEA Saclay	France	jean-luc.bechade@cea.fr
BERGER	Rosabelle	CEA Saclay	France	rosabelle.berger@cea.fr
CHARTIER	Alain	CEA Saclay	France	alain.chartier@cea.fr
CHROMIŃSKI	Witold	NCBJ (NOMATEN)	Poland	witold.chrominski@pw.edu.pl
CLOUET	Emmanuel	CEA Saclay	France	emmanuel.clouet@cea.fr
CROCOMBETTE	Jean-Paul	CEA Saclay	France	jpcrocombette@cea.fr
DOLLÉ	Frédéric	CEA Saclay	France	frederic.dolle@cea.fr
DOMINGUEZ GUT.	Frans. Javier	NCBJ (NOMATEN)	Poland	javier.dominguez@ncbj.gov.pl
DROZD	Maciej	NCBJ (NOMATEN)	Poland	maciej.drozd@ncbj.gov.pl
DUPUY	Laurent	CEA Saclay	France	laurent.dupuy@cea.fr
ESFANDIARPOUR B.	Amin	NCBJ (NOMATEN)	Poland	amin.esfandiarpour@ncbj.gov.pl
FAN	Zhengxuan	CEA Saclay	France	zhengxuan.fan@cea.fr
FRELEK-KOZAK	Malgorzata	NBCJ (NOMATEN)	Poland	malgorzata.frelek-kozak@ncbj.gov.pl
FRYDRYCH	Karol	NCBJ (NOMATEN)	Poland	karol.Frydrych@ncbj.gov.pl
GALLÉ	Christophe	CEA Saclay	France	christophe.galle@cea.fr
HODILLE	Étienne	CEA Grenoble	France	etienne.hodille@gmail.com
HURE	Jérémy	CEA Saclay	France	jeremy.hure@cea.fr
JAGIELSKI	Jacek	NCBJ (NOMATEN)	Poland	jacek.jagielski@ncbj.gov.pl
JÓŹWIK	Iwona	NCBJ (NOMATEN)	Poland	iwona.jozwik@ncbj.gov.pl
KARIMI	Kamran	NCBJ (NOMATEN)	Poland	kamran.karimi1362@gmail.com
KARLSEN	Wade	VTT	Finland	wade.karlsen@vtt.fi
KOMOROWSKI	Maciej	NCBJ (NOMATEN)	Poland	maciej.Komorowski@ncbj.gov.pl
KOTIPELTO	Arto	VTT	Finland	arto.kotipelto@vtt.fi
KOSIŃSKA	Anna	NCBJ (NOMATEN)	Poland	anna.Kosinska@ncbj.gov.pl
KURPASKA	Łukasz	NCBJ (NOMATEN)	Poland	lukasz.kurpaska@ncbj.gov.pl
KRZYCZMONIK	Anna	NCBJ (NOMATEN)	Poland	anmakrz@utu.fi
LAHAYE	Cjolé	CEA Saclay	France	chloe.lahaye@cea.fr
LINDQVISTE	Sebastian	VTT	Finland	sebastian.lindqvist@vtt.fi
LINDROOS	Matti	VTT	Finland	matti.lindroos@vtt.fi
LOYER-PROST	Marie	CEA Saclay	France	marie.loyer-prost@cea.fr
MADELAIN	Martin	CEA Saclay	France	martin.madelain@cea.fr
MARINICA	Cosmin	CEA Saclay	France	mihai-cosmin.marinica@cea.fr
MARTINELLI	Laure	CEA Saclay	France	laure.martinelli@cea.fr
MOUTIERS	Gilles	CEA Saclay	France	gilles.moutiers@cea.fr
MULEWSKA	Katarzyna	NCBJ (NOMATEN)	Poland	katarzyna.mulewska@ncbj.gov.pl
NASTAR	Maylise	CEA Saclay	France	maylise.nastar@cea.fr

Modeling of the behaviour of materials under irradiation

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

List of participants (2/2)

Family Name	First Name	Company	Country	e.mail
OLEJARZ	Artur	NCBJ (NOMATEN)	Poland	artur.olejarz@ncbj.gov.pl
NORI	Sri Tapaswi	NCBJ (NOMATEN)	Poland	sritapaswi2007@gmail.com
OKSA	Maria	VTT	Finland	maria.oksa@vtt.fi
ONIMUS	Fabien	CEA Saclay	France	fabien.onimus@cea.fr
PAPANIKOLAOU	Stefanos	NCBJ (NOMATEN)	Poland	stefanos.papanikolaou@ncbj.gov.pl
POISVERT	Axel	NCBJ (NOMATEN)	Poland	axeleliott.poisvert@gmail.com
PROUILHAC	Christine	CEA Saclay	France	christine.prouilhac@cea.fr
PRUSZYŃSKI	Marek	NCBJ (NOMATEN)	Poland	marek.pruszynski@ncbj.gov.pl
REN	Sicong	VTT	Finland	sicong.ren@vtt.fi
ROVARIS	Fabrizio	NCBJ (NOMATEN)	Poland	fabrizio.rovaris@ncbj.gov.pl
SIPILÄ	Konsta	VTT	Finland	konsta.Sipila@vtt.fi
SOBCOWICZ	Pawel	NCBJ (NOMATEN)	Poland	pawel.sobkowicz@ncbj.gov.pl
SUCHORAB	Kinga	NCBJ (NOMATEN)	Poland	kinga.Suchorab@ncbj.gov.pl
TALLA NOUTAK	Martin Sté.	CEA Saclay	France	martin.talla@cea.fr
TOFFOLON	Caroline	CEA Saclay	France	caroline.toffolon@cea.fr
VAN BRUTZEL	Laurent	CEA Saclay	France	laurent.vanbrutzel@cea.fr
VEPSÄLÄINEN	Mikko	VTT	Finland	mikko.vepsalainen@vtt.fi
WILCZPOLSKA	Magdalena	NCBJ (NOMATEN)	Poland	magdalena.wilczopolska@ncbj.gov.pl
ZABOROWSKA	Agata	NCBJ (NOMATEN)	Poland	agata.Zaborowska@ncbj.gov.pl
ZIELIŃSKI	Maciej	NCBJ (NOMATEN)	Poland	maciej.zielinski@ncbj.gov.pl

More informations ?

http://nomaten.ncbj.gov.pl/winterschool2021