Cargese, Corsica, France
September 24 – October 6, 2007

NATO Advanced Study Institute

Materials for Generation IV Nuclear Reactors

Application deadline: June 15, 2007

Full registration fee: 800 €, scholarships available upon demand to: matgen@cea.fr

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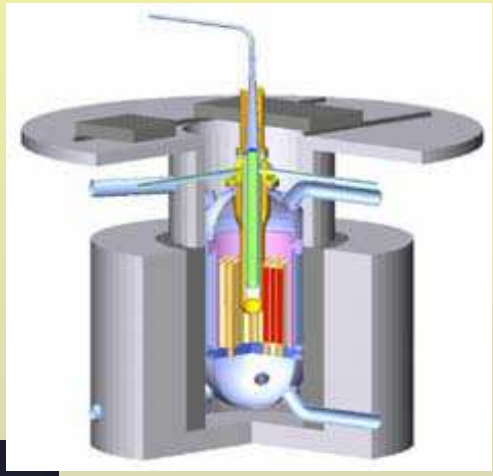
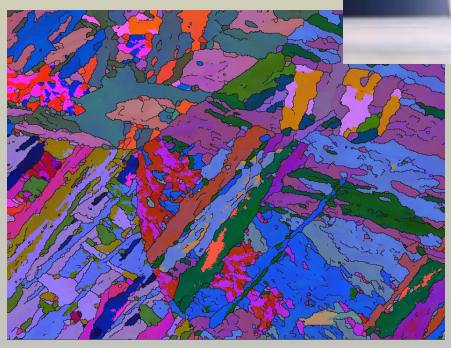




TOPICS

- Energy Issue and scenarios studies
- Non-proliferant generation IV systems
- Neutronics and safety
- Thermodynamics (equilibrium and non-equilibrium phase diagrams)
- Particle/matter interaction
- Structure materials (from steels to ceramics)
- Radiation effects : from atomic to macroscopic scale
- Fracture: statistical and metallurgical approaches
- Multi-scale computer simulations
- Liquids: fundamentals, coolant properties and control
- Interfaces, segregation and wetting
- HTR, liquid metal and molten salt reactor concepts
- Physics of spallation and applications to incineration of long lived radioactive wastes in ADS

ORGANIZERS

CEA : A. Alamo, P. Chaix, D. Mazière, V. Pontikis
CNRS : V. Ghetta, D. Gorse
KIP : A. Bakai
KTH : J. Wallenius

List of lecturers and information available on:
http://www-matgen4.cea.fr

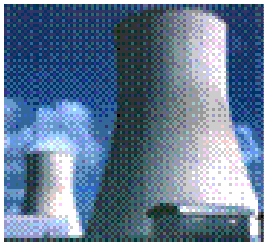
ESM, Écoles en Sciences des Matériaux

GEDÉPÉON, Gestion des Déchets et Production d'Énergie par des Options Nouvelles

SUMMARY

G – LECTURES

In lecturers order



H – POSTERS

In authors order

A - THANKS

The NATO Advanced Study Institute MATGEN IV will be introduced by Jean-Pierre Le Roux, vice chairman of the Atomic Energy Commission who will find here our warmest thanks for having joined us to welcome the participants and to open this outstanding event.

We would like to greatly acknowledge all the sponsors listed below and more particularly the NATO responsible persons for 'Science for Peace and Security Programme' for their substantial financial support and efficient help (particularly Alison Trap).

Many thanks too, to Laurent Turpin, Constantin Meis and Joseph Safieh from the National Institute of Nuclear Sciences and Techniques (CEA) for having accepted the active Institute's involvement and to Aurore Rodier for the preparation of all the documents related to the school and for the forthcoming work in September in Cargese.

Our acknowledgements will go also to the National Center for Scientific Research, and especially Mme Gilberte Chambaud, Director of the Chemistry Department, and Mr. Patrick Seta, "chargé de mission formation" from the Chemistry Department for their interest in this project, from its very beginning.

This booklet contains the abstracts of the lectures, seminars and posters that will be presented during the NATO ASI. The Organizers wish to thank the authors for their contribution and their help during the preparation of the School. Moreover, the hard work of our colleagues involved in the organization of the Practical Sessions is warmly acknowledged.

At last, the Organizers would like to express their gratitude to Mme Elisabeth Dubois-Violette, Director of the Institut d'Etudes Scientifiques de Cargèse, who accepted to host MATGEN-IV at the IESC.

The organizing committee thanks all the participants for their confidence and wish to all of them a very fruitful and pleasant stay in Cargèse.

The organizers

B - SPONSORS AND SUPPORT

Organizations:

- North Atlantic Treaty Organization (NATO)
  Science for Peace and Security (SPS)
- Commissariat à l'Energie Atomique (CEA)
  - Direction de l'Energie Nucléaire - Département des Matériaux Nucléaires (DEN/DMN)
  - Direction des Sciences de la Matière - Département de Recherche sur les Atomes et les Molécules (DSM/DRECAM)
  - Institut National des Sciences et Techniques Nucléaires (INSTN)
- Centre National de la Recherche Scientifique (CNRS)
  - Centre d'Etudes de Chimie Métallurgique (CECM)
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- Electricité de France - EDF
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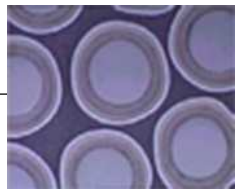
Other Sponsors:

- European Nuclear Education Network association (ENEN)

C - OBJECTIVES AND COMMITTEES



Objectives

This advanced school focuses on the identification of the new structural materials that will be needed for Generation-IV nuclear reactors, and on the methodology required for their development. In a series of lectures and seminars the required fundamental knowledge on relevant material properties will be presented, together with methodological tools and processing techniques. The use of theoretical, computational and experimental tools will be presented in detail during practical exercises (e.g. computation and assessment of phase diagrams) while round tables and poster sessions will provide several opportunities for general exchanges intended to foster future collaborations among participants.

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Prof. J. Wallenius	KTH, Stockholm, Sweden

Institut d'Etudes Scientifiques de Cargese

Menasina beach

Péro Beach

E - SCHEDULE

First week

25/09	09H00-09H30	WELCOME
	09H30-10H00	Opening speech by JP. Le Roux, vice chairman of the Atomic Energy Commission.
	10H00-11H00	The energy issue and the possible contribution of the various nuclear energy production scenarios, H. Nifenecker
	11H30-12H30	Introduction to thermodynamics, G. Inden
	14H30-15H30	Outlook on Generation IV Nuclear Systems and related materials R&D challenges, F. Carré
	15H30-16H30	Introduction to neutronics, JM. Cavedon
	17H00-18H00	Particle/matter interaction in the keV-MeV range, E. Balanzat
26/09	08H30-9H30	Energy production scenarios; emphasis on safety, non – proliferation aspects and consequences on materials, H. Nifenecker
	09H30-10H30	Kinetics of phase transformations in multi-component systems, G. Inden
	11H00-12H00	Fundamentals of neutronics: reactivity coefficients of nuclear reactors, P. Reuss
	14H30-15H30	Fundamentals of neutronics: reactivity coefficients of nuclear reactors, P. Reuss
	15H30-17H00	A First-Principles Approach to Designing Materials, A. Pasturel
	17H30-18H30	ROUND TABLE : Safe, reliable, robust and non-proliferant generation IV systems
27/09	08H30-10H30	Fracture mechanisms, P. Spatig
	11H00-12H00	Fracture mechanisms and scaling properties of fracture surfaces, E. Bouchaud
	14H30-15H30	Particle/matter interaction in the keV-MeV range, E. Balanzat
	15H30-16H30	Numerical modeling of radiation effects in solids: principal features, limitations and perspectives, P. Geysermans
	17H00-18H00	Correlation between electronic structure, magnetism and physical properties of Fe-Cr alloys: ab initio modelling, I. Abrikosov
	18H00-19H00	Practical Session-1: Equilibrium phase diagrams, G. Inden/MN. de Noirefontaine
28/09	08H30-09H30	Crystal plasticity from Dislocation Dynamics, V. Bulatov
	09H30-10H30	Microstructural and mechanical properties of irradiated structural materials, S. Zinkle
	11H00-12H00	Microstructural and mechanical properties of irradiated structural materials, S. Zinkle
	14H30-15H30	Microstructural and mechanical properties of irradiated structural materials, S. Zinkle
	15H30-16H30	Radiation-induced solute segregation and precipitation in alloys, A. Ardell
	17H00-18H00	Parametric dislocation dynamics and boundary element modeling of elastic interaction dislocations/precipitates, A. Takahashi
	Poster Session-1	
29/09	08H30-09H30	The Computational Modeling of Alloys at the Atomic Scale: From Ab Initio and Thermodynamics to Radiation-Induced Heterogeneous Precipitation, A. Caro
	09H30-10H30	Multiscale computer simulations and predictive modeling of RPV embrittlement, N. Soneda
	11H00-12H00	Multiscale computer simulations and predictive modeling of RPV embrittlement, N. Soneda
	14H30-15H30	Presentation of the toughness module from the Perfect project, S. Bugat
	15H30-16H30	Kinetic Monte Carlo simulations of radiation damage in structural materials, P. Ollson
	17H00-18H00	Practical Session-2: Electronic structure calculations in iron with defects (formation and migration energies) and/or gases (interaction vacancy – helium atoms), Chu Chun Fu/G. Lucas

Second week

01/10	08H30-09H30	Neutrons and radiation damage in structural materials, J. Wallenius
	09H30-10H30	SiC as a material for application in generation IV systems: electronic, structural and mechanical properties, P. Pirouz
	11H00-12H00	SiC as a material for application in generation IV systems: electronic, structural and mechanical properties, P. Pirouz
	14H30-15H30	Chemical compatibility of SiC composite structures with GFR helium at high temperatures – bibliographic review, C. Cabet
	15H30-16H30	The Effects of Irradiation Damage in Structural Ceramics, L. Snead
	17H00-18H00	PrS-2 (continued): Ab-initio calculation of defect properties in SiC, Chu Chun Fu/G. Lucas
02/10	08H30-10H30	Fundamentals of liquids, JP. Hansen
	11H00-12H00	Fundamentals of Interfaces, P. Wynblatt
	14H30-15H30	Fundamentals of Interfaces, P. Wynblatt
	15H30-16H30	Wetting, D. Chatain/V. Ghetta
	17H00-18H00	Thermophysical properties of liquid metals and alloys, an experimental approach, G. Pottlacher
03/10	08H30-09H30	Fundamentals of liquids, JP. Hansen
	09H30-10H30	Wetting, D. Chatain/V. Ghetta
	11H00-12H00	Liquid sensors: principles and measurements, J. Fouletier/V. Ghetta
	14H30-15H30	Influence of Liquid Sodium on mechanical properties of steels, refractory alloys and ceramics. Part 1: Corrosion and Reactions with Impurities Dissolved in Sodium, H. Borgstedt
	15H30-16H30	Chemistry control in large installations: requirements, purification strategies, system design, C. Latgé
	17H00-18H00	Liquid metal embrittlement, V. Pontikis/D. Gorse/V. Ghetta
	18H00-19H00	Poster Session-2
04/10	08H30-09H30	Influence of Liquid Sodium on mechanical properties of steels, refractory alloys and ceramics - Part 2: Creep Rupture and Low Cycle Fatigue of Reactor Materials in Liquid Sodium, H. Borgstedt
	09H30-10H30	Structural Materials for Fusion Power Plants - Part I: Radiation Effects and Major Issues, JL. Boutard
	11H00-12H00	Operation of high power liquid metal spallation targets: a challenge for the structural materials, J. Henry
	14H30-16H30	Research and Development of ODS Ferritic Steels for Sodium Cooled Fast Breeder Reactor Fuels, M. Inoue
	17H00-18H00	Structural Materials for Fusion Power Plants - Part II: Multi-scale Modelling Radiation Effects, JL. Boutard
	18H00-19H00	ROUND TABLE: Materials issues for generation IV systems
05/10	08H30-09H30	Introduction to the physics of molten salt reactors, E. Merle
	09H30-10H30	Physical and chemical properties of molten salts, JC. Poignet
	11H00-12H00	Combined effect of molten fluoride salt and irradiation on Ni-based alloys, A. Bakaï
	14H30-16H30	Specific features of particule/matter interaction for accelerator-driven sub-critical reactors, S. Leray
	17H00-18H00	Liquid sensors: application to heavy liquid metals, J. Fouletier
06/10	09H00-10H00	Future prospects for periodic schools on this topic.

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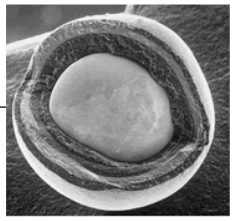

GL1-1

The energy issue and the possible contribution of the various nuclear energy production scenarios

H. Nifenecker
France

In the inaugural lecture of this school, the energy issue is presented. The main ingredient, demographic as well as economic, of energy consumption scenarios, are described. The worldwide energy needs based on present and future consumptions of energy will be presented for several plausible scenarios, with special reference to those of the IAASA-WEC.
The non - nuclear energy sources (coal, fuel, gas, renewable…), their perspective of growth, including the state of their reserves, and their impact on the climatic evolution, are reviewed. Different electric energy production scenarios are detailed, with various contributions of nuclear power. The interest of a new deployment of nuclear power in the world be discussed.

GS-1

Introduction to Thermodynamics

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It is the aim of the course to give a comprehensible introduction into the field of thermodynamics. Starting from the principles, the fundamental concepts and their mathematical formulations will be introduced: integral quantities like various forms of exchanged energies, partial molar quantities like chemical potentials, activities etc.. The emphasis will be placed on chemical thermodynamics dealing with multi-component systems of solid, liquid and gaseous phases. The thermodynamic description of multi-component solution phases is presented and applied to obtain stable and metastable multiphase equilibria, driving forces for reactions etc... Various types of diagrams will be introduced and their use for solving practical problems will be illustrated. The illustration of examples will be based on numerical techniques that are nowadays available and are being used both in academic research and in industry.

GL2

Outlook on Generation IV Nuclear Systems and related materials R&D challenges

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The fast growing energy demand driven by the increasing world population and the development of China and India, together with recognized assets of nuclear energy in terms of energy security and limitation of greenhouse gas emission have led since 2000 to acknowledge the role that nuclear energy ought to play among other energy sources to satisfy future energy needs of mankind. Generation III light water reactors (LWRs), which materialize optimized versions of current nuclear generating facilities, are anticipated to develop actively in both above large populated countries as well as to replace or augment existing nuclear power plants in already equipped countries. Beyond the commercialization of best available light water reactor technologies, it is essential to start now developing breakthrough technologies that will be needed to prepare the longer term future for nuclear power to represent a significant share of energy production in the 2nd half of the 21st century and beyond:

- ***Fast neutron reactors with a closed fuel cycle*** which afford making an efficient use of uranium resource (more than 80% instead of 1% at most by light water reactors which essentially consume ^{235}U) and minimizing long-lived radioactive waste, thus making nuclear energy more sustainable, and
- ***High temperature reactors*** that may drive more efficient processes to generate other energy products than electricity such as hydrogen, synthetic hydrocarbon fuels from coal or biomass, or process heat for the industry, thus contributing to enlarge the range of applications of nuclear energy.

Several initiatives today such as the Generation IV International Forum and the IAEA International Project on Innovative Nuclear Reactor (INPRO) aim today at revisiting the technologies that led to early prototypes of reactors of both above types, and to search for innovations that could make them progress significantly in competitiveness, safety and operability so as to prepare the development of attractive commercial nuclear systems. Fast reactors are expected to be needed around 2040 if, as anticipated today, the installed capacity of LWRs reaches 1300-1500 GWe by 2050, and uranium prices escalate because most of the estimated resource below 130 $/kg (i.e. ~15 Mtonnes) is preempted by fueling needs of these reactors over a 60-year lifetime. Moreover, if their technical maturity and competitiveness arise earlier, fast neutron reactors could support the industrial implementation around 2030 of the Global Nuclear Energy Partnership's strategy that is proposed by the US-DOE to safely develop nuclear power worldwide with an adequate control of proliferation risks. This strategy is based on a practice of nuclear fuel leasing and take-back services assured by "fuel-cycle states" that would operate such fast neutron reactors to recycle nuclear materials recovered from retrieved LWR spent fuel.

For either of both above applications, fast neutron reactors are being revisited along basically three tracks: innovative sodium cooled fast reactors (SFRs) that are likely to lead to prototypes around 2020-25 and be ready for industrial deployment by 2040 or earlier, and alternative technologies, gas or lead-alloy cooled fast reactors (GFRs and LFRs), that call for experimental technology demonstrators around 2020 prior to considering prototypes around 2030-35, and industrial deployment after 2050.

Besides, high temperature reactor (V/HTR) energy products might become marketable as early as 2025, especially to oil and refinery companies that need high temperature process heat and hydrogen already today and possibly synthetic hydrocarbon fuels from coal or biomass to complement fuels from fossil origin.

Key technologies for such Generation IV nuclear systems encompass high temperature structural materials, fast neutron resistant fuels and core materials, advanced fuel recycle processes with co-management of actinides, possibly including minor actinides, and specific reactor and power conversion technologies *(intermediate heat-exchanger, turbo-machinery, high temperature electrolytic or thermo-chemical water splitting processes…).*

The paper will give a brief overview of various materials that are key for above nuclear systems' feasibility and performance:

- ***Ferritic/Martensitic steels*** (9-12% Cr) are promising candidate materials for sodium cooled reactors with a high temperature (<600℃) and compact primary system, as well as for the pressure vessel of high temperature gas-cooled reactors
- ***Nickel based alloys*** (Haynes 230, Inconel 617…) are promising candidate materials for high temperature gas-cooled primary system's components such as the intermediate heat exchanger, and oxide dispersion strengthened grades are considered to match requirements for higher temperature service conditions (intermediate heat exchanger, gas turbine blades…)
- ***Oxide dispersion strengthened ferritic / martensitic steels*** are promising candidates as cladding materials for high burn-up fast neutron reactor fuels
- ***Ceramic materials*** are needed for very high temperature components (> 1000℃) such as heat exchangers and thermal insulations in the primary system, as well as core components such as control rod sheath (V/HTR and GFR) and fuel constituents (GFR), with a major effort of research being invested in developing less brittle ceramics forms such as composite ceramics, nano-structured plastic ceramics… SiC, that has been extensively investigated for Fusion applications, is the major focus of R&D today but other carbides (TiC, ZrC) or nitride (TiN, ZrN…) are also currently considered in screening tests. Ceramics are also needed for parts of power conversion systems such as very high temperature gas turbine blades or intermediate heat exchangers to decompose sulfuric acid (> 850℃) as high temperature step of several thermo-chemical water splitting processes *(iodine-sulfur, Westinghouse hybrid…)*
- Other specific materials such as up-to-date grades of ***graphite*** for V/HTRs.

The paper will also give an insight into the various natures of R&D needed on advanced materials, including fundamental research to investigate basic physical and chemical phenomena occurring in normal and accidental operating conditions, multi-scale modeling to predict macroscopic materials properties and to direct innovative research for improvements, lab-scale tests to characterize candidate materials mechanical properties and corrosion resistance, as well as component mock-up tests on technology loops to validate potential applications while accounting for mechanical design rules and manufacturing processes.

Finally, the paper will stress the benefit of prospects of multilateral collaboration within the Generation IV International Forum and the 7th European R&D Framework Program to join skills and share efforts of R&D to achieve in the nuclear field breakthroughs on materials that have already been achieved over the past decades in other industry sectors *(aeronautics, metallurgy, chemistry…).*

Introduction to neutronics

J-M. Cavedon

Particle-matter interaction in the keV-MeV range

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This lecture concerns the basic physical processes underlying the defect production in irradiated solids.

A comprehensive picture of the radiation damage needs to consider very different scales: nuclear, atomic and solid-state. Nuclear reactions giving secondary particles were not addressed here, as they are presented in a specific lecture. The slowing down of particles in matter is usually treated at the atomic level by considering a two-body collision between the projectile and atom of the solid. These atomic collisions mainly govern the fate of the projectile. However, the solid state scale has, in some cases, a significant incidence: for instance in the channelling process and in the charge state distribution of ions penetrating solids. Evidently, the damage process itself is governed by the solid characteristics.

The atomic collision is generally described by distinguishing the interaction with the electrons of the atom and the atom itself. This gives rise to the so-called electronic (or inelastic) and nuclear (or elastic) stopping powers. We present the different approaches used for calculating these values and give their relative importance for different radiation situations.

The irradiating projectiles induce primary knock-on particles (electrons or atoms). But for describing the energy deposition in the solid the fate of secondary (and higher) particles is essential. Therefore, the development of atomic or electronic cascades is presented. We show, for typical irradiation facilities, the characteristic of the primary-recoil spectrum and their characteristic integral values and we discuss the basis of the experimental simulation with accelerator beams of the complex radiation fields occurring in real life.

The consequences in term of damage of the two stopping processes are very different: direct transfer of kinetic energy to target atoms for the elastic stopping and transient perturbation of the electronic structure for the inelastic stopping. Consequently, the response of the solid to the inelastic or elastic perturbation is very material dependent. The other crucial parameter is the magnitude of the perturbation. Schematically, this leads to four different situations (elastic or inelastic and low or strong perturbation): i) when the kinetic energy transferred to an individual atom (the primary recoil or PKA) is low, we are within the domain of Frenkel-pair creation or in the regime of linear cascades ii) low electronic stopping powers corresponds to classical radiolysis conditions iii) higher PKA energies could induce non-linear cascades when atoms put in movement collide with atoms that are still moving iv) high electronic stopping could induce track formation. For different materials metallic or not, we present the damage processes in these four different situations, putting emphasis on the effects of the elastic stopping. Possible interactions between electronic and elastic stopping are evoked.

GL1-2

Energy production scenarios; emphasis on safety, non – proliferation aspects and consequences on materials selection

H. Nifenecker, France

In this second lecture devoted to the energy issue the nuclear energy production scenarios are detailed. The status of uranium natural and thorium resources, considering today and possible future level of resource are presented. Needs for spent fuel reprocessing, are discussed. Based on both the electric energy needs and the available resources, various schemes of deployment of nuclear power plants are presented. They are analysed taking into consideration the requirements of sustainability, safety, reliability and proliferation resistance. The different options of the GEN IV initiative are briefly presented (SFR, LFR, GFR, MSR…). In this frame the needs for new material and corrosion studies are stressed.

GS-2

Kinetics of phase transformations in multi-component systems

G. Inden, FZK, Germany

The mechanical properties of materials are controlled by the microstructure, which is obtained by an adequate heat treatment. This treatment determines a first time scale which, in the case of steels, is often too short to yield equilibrium. If the material is then subjected to long - term service conditions at higher temperatures, the microstructure changes, leading to a deterioration of the mechanical properties. It is thus important to know about the kinetics of these reactions. Furthermore, it is by no means granted that only those phases have to be considered which are present at equilibrium. Metastable phases may kinetically be favoured in comparison to stable phases such that, at intermediate stages, metastable phases also appear in the microstructure. These phases will eventually disappear, but their temporary existence influences strongly the kinetics of formation of the microstructure. It is thus important to know about their occurrence and their life time in the microstructure.

The various thermodynamic aspects of growth kinetics of stable and metastable phases in steels will be treated. Particular emphasis will be placed on criteria for fast and slow reactions which can be used either to solicit the appearance of wanted precipitates or to inhibit the precipitation of unwanted phases. In this context, the thermodynamic aspects of the growth conditions of phases like $M_{23}C_6$, M_7C_3, M_3C, M_6C and Laves phase will be discussed with model alloys based on Fe-Cr-C-X. With computer simulations it is possible to provide quantitative information on the transformation kinetics, in particular for long-term applications. The results show remarkable effects on the growth kinetics due to competition of stable and metastable phases during simultaneous growth.

GS2

Fundamentals of neutronics: reactivity coefficients of nuclear reactors

P. Reuss, CEA-Saclay

It is of course impossible to present neutronics in one or two hours. This lecture will be therefore restricted to the analysis of the basic physic principles of the fission-neutron chain reaction and to the examination of the main characteristics of a nuclear reactor behaviour.

Particularly, the aspects concerning, from the neutronics point of view, the choices of the materials – theme of this summer school – will be emphasized : main options for the core design, reactivity effects, conditions for a working stability, neutron utilization.

The coupling between the neutronics and the other branches of physics involved in the reactor design – thermal-hydraulics, irradiation of materials, safety… – will be rapidly discussed in the conclusions.

A First-Principles Approach to Designing Materials

A. Pasturel (CNRS - Grenoble Institute of Technology (INPG*)*

The role of basic energetic and thermodynamic data in designing new materials is crucial towards their application. Fundamental knowledge of the microscopic factors governing alloy phase stability has increased greatly due to the development of highly-accurate “state-of-the-art” fist principles computational approaches and recent works have demonstrated substantial quantitative improvements in the accuracy of alloy phase diagrams calculated by these techniques.
We will present an overview of recent developments in the application of first-principles calculations to the study of thermodynamic properties and phase equilibria in materials for nuclear applications. Our presentation will be illustrated by applications to the modelling of phase diagrams in metallic systems (Zr- and Pu- based alloys) and the structural stability of UO_2 under irradiation.
We will also discuss how this parameter-free methodology can play a central role in predicting new classes of materials with targeted properties, designed on computers rather than in laboratories

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ML1/S1

A Multi-scale Approach to Understanding the $K_{Jc}(T)$ Brittle to Ductile Cleavage Transition in Ferritic Alloys

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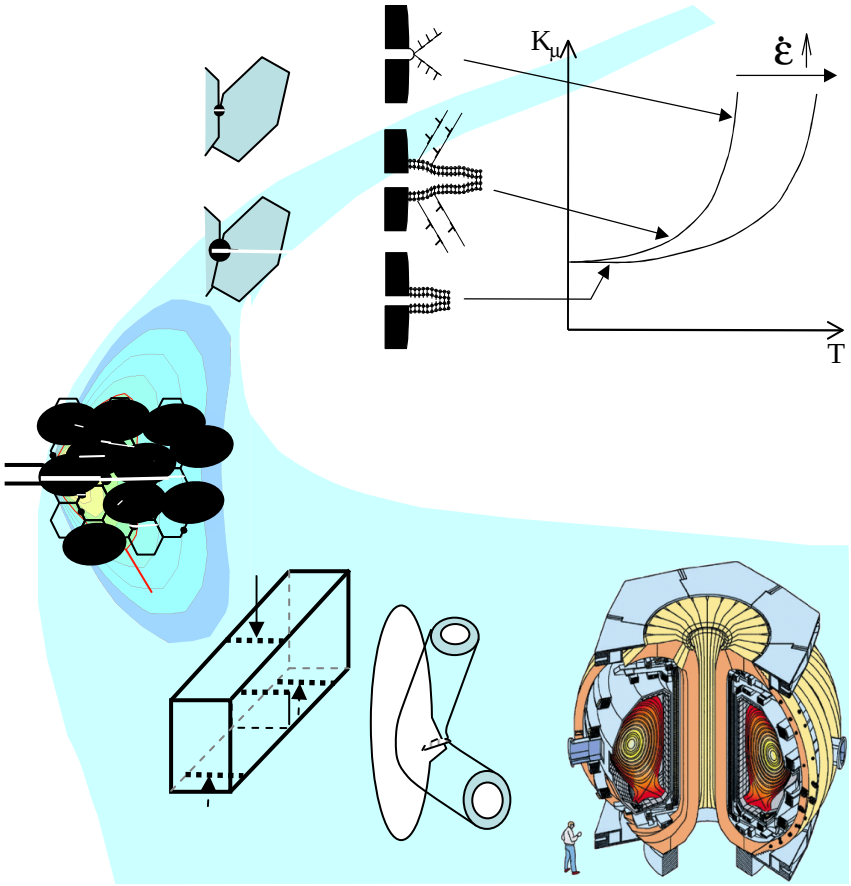

DRAFT - Extended Abstract

A Multi-scale Approach to Understanding the $K_{Jc}(T)$ Brittle to Ductile Cleavage Transition in Ferritic Alloys

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Our lecture overviews the physical processes that mediate cleavage fracture toughness from atomic to structural length scales. After a brief review of the 'local approach' to fracture, we use open questions about the so-called master curve method (MCM) as a framework to address cleavage mechanisms and models [1-5]. The MCM is based on the empirical observation that the toughness temperature $K_{Jc}(T-T_o)$ curves of steels seem to have a remarkably invariant master curve (MC) shape, while the reference temperature, T_o, varies over a wide range, depending on the material microstructure and test conditions. Our objective is to understand and quantitatively model: 1) the shape of the toughness-temperature master curve over a wide range of T_o; 2) the effects of cracked body size, geometry on fracture toughness in the cleavage transition; and 3) loading rate and irradiation induced T_o shifts. These the fracture properties are linked to the material constitutive and local fracture properties and, hence, also to the underlying alloy microstructure.

For unirradiated alloys, with $T_o < 0℃$, an invariant MC shape is predicted by simple micromechanical models, assuming cleavage fracture occurs when an approximately temperature independent critical stress (σ^*) contour encompasses a critical local volume (V^*) of material in front of a blunting crack tip [4,5]. Continuum finite element (FE) methods are used to determine the loading (K_{Jc}) at cleavage as mediated by the alloy's constitutive properties and local fracture properties, σ^* and V^*. At low T_o the shape of $K_{Jc}(T)$ is governed almost entirely by the temperature dependence of $\sigma_y(T)$. However, irradiation hardening, $\Delta\sigma_y$, increases T_o (ΔT_o) which may reach values of more than 200℃. When T_o is in the athermal regime, where σ_y only weakly depends on temperature, the assumption of a temperature independent σ^* predicts changes (layovers) in the shape of $K_{Jc}(T)$. This apparent contradiction with observation is resolved by a mildly temperature dependent $\sigma^*(T)$ at higher temperatures. The $\sigma^*(T)$ temperature dependence is, in turn, controlled by the micro-arrest toughness of the material controlling the conditions for the propagation of dynamic microcracks formed at brittle trigger particles in the high stress region of the crack tip process zaone. We hypothesize that the temperature dependence of micro-arrest toughness is controlled by atomic scale processes, and that this valves the much higher $K_{Jc}(T)$ toughness at larger length scales, thus leading to an invariant MC shape.

In pursuit of independent support this hypothesis, we describe results of a recent experimental study of the temperature dependent initiation (K_{Ic}) and arrest toughness (K_a) of cleavage oriented (100)[010] and (100)[011] Fe single crystals, using specially designed composite specimen test techniques [6]. The $K_a(T)$ is weakly temperature dependent below about -100℃, increasing from a minimum of 3.5 MPa $\sqrt{m}$, but rises more rapidly to 9 MPa$\sqrt{m}$ at higher temperatures near 0℃.

Static and dynamic single crystal $K_{Ic/d}(T)$ curves were also measured over a wide range of loading rates from about 0.1 to 20,000 MPa$\sqrt{m}$/s. In all cases, *the cleavage fracture dynamics were found to be controlled by nucleation of double kinks on screw dislocations, that also controls the flow stress dynamics.* When plotted on a strain rate compensated temperature, T', the arrest and initiation data overlap to form a $K_a(T')$ master curve.

The single crystal results were extended complex alloys by proposing that both the thermal and athermal contributions to σ_y combine to control $K_a(T)$ [unpublished]. The interplay between K_a and σ_y is represented by a simple model $K_a(T')\sigma_y(T) = C(\sigma_y)$, with a minimum polycrystalline K_a of about 3.5 MPa, where $C(\sigma_y)$ is fitted to the single crystal data at -196℃ and is a weak function of σ_y. Using $K_a(T) = C(\sigma_y)/\sigma_y(T)$ curves in the macroscopic $K_{Jc}(T)$ model results in approximate master curve shapes over a wide range of T_o.

We also show the model properly predicts ΔT_o due to irradiation and high strain rate induced increases in the average alloy flow stress between 0 and 10% plastic strain, $\Delta\sigma_{fl}$, with a typical $\Delta T_o/\Delta\sigma_{fl} \approx 0.7$℃/MPa [3,4,7]. The use of $\Delta\sigma_{fl}$, rather than $\Delta\sigma_y$, accounts for the loss of strain hardening due of irradiation [7]. Finally, the fracture toughness both pertinent to structures and measured using small test specimens always depends on the size and geometry of the cracked body. Size and geometry effects arise from both statistical probabilities, related to the volume under high stress near a crack tip, and constraint loss associated with large amounts of deformation in small specimens and in the case of shallow surface cracks in structures. We describe micromechanical models that can be used to adjust the toughness measured using small specimens to both the intrinsic material K_{Jc} and the effective toughness pertinent to a structure [8,9].

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Fracture mechanisms and scaling properties of fracture surfaces

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For very different materials, the morphology of fracture surfaces reveals anisotropic scale invariance properties which can be described with two sets of parameters: roughness exponents and characteristic length scales, measured either along the direction of crack propagation, or perpendicularly to it. If characteristic length scales depend on the material, its microstructure, and the external loading, roughness exponents, on the contrary, are “universal”. However, several classes of universality reflect various fracture modes.

Sintered glasses, which break in a perfectly elastic manner, exhibit a certain set of roughness exponents. Their fracture surfaces were recently shown to be captured within the framework of a stochastic equation describing crack front deviations and pinning by microstructural disorder.

But the roughness exponents observed for example for metallic alloys and for glasses, albeit at length scales three orders of magnitude smaller in the latter case, are significantly different. This difference is suggested to originate in the presence of a damage zone ahead of the main crack front, where roughness measurements are actually performed. Atomic Force Microscopy experiments on silicate glasses show indeed damage formation ahead of a stress corrosion crack tip over several hundreds of nanometers, while fracture surface roughness measurements are limited to one hundred nanometers. The critical exponents observed in this case, as well as in the case of metallic materials, are conjectured to reflect damage screening occurring at length scales smaller than the process zone size.

Very recent results on the structure of damage cavities in metallic glasses are also discussed.

GL6

Numerical modeling of radiation effects in solids: principal features, limitations and perspectives

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The non-linear and far from the thermodynamic equilibrium phenomena triggered in solids under irradiation result in the formation of history-dependent microstructures controlling their physical properties. All these features together render the theoretical approach difficult so that computer modeling appears as the unique methodology available to assist experiments and to help de-convoluting the results.

This presentation first focuses on atomistic computer modeling with special emphasis on the achievements of this approach as well as on its limitations, the associated space and time scales. These are the principal motivations for the development of a multiscale approach ideally consisting in a succession of models its providing input information to the model acting at the immediate next time and space scales. The methodologies used to bridge the gap between multiple space and time scales are briefly reviewed together with difficulties encountered preventing the approach from being predictive. We conclude suggesting perspectives of improvement and development of modeling methods in irradiation phenomena.

Correlation between electronic structure, magnetism and physical properties of Fe-Cr alloys: ab initio modeling

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We review recent developments in the field of *ab initio* electronic structure theory and its application for studies of complex alloy systems. Basic ideas behind state-of-the-art techniques for first-principles theoretical simulations of the phase stabilities and properties of intermetallic compounds and alloys based on the density functional theory are outlined. We concentrate on methods that allow for an efficient treatment of disorder effects [1,2], and illustrate their predictive power for the case of Fe-Cr system.

In the binary Fe-Cr alloy the decomposition occurs either via the nucleation and growth mechanism or as spinodal decomposition, depending on the Cr content. However, at low chromium concentrations the alloys are anomalously stable. This is shown to be true only for the ferromagnetic body centered cubic (bcc) phase[3,4]. Indeed, we show that in the paramagnetic alloys the concentration dependencies of the thermodynamic properties are smooth functions of alloy concentration, in agreement with the high-temperature experiment. However, in the ferromagnetic case there are peculiarities of the mixing enthalpy and bulk moduli in the low-Cr region in the bcc phase. We show that the stability of the low-Cr steels stems from the negative mixing enthalpy at low concentrations of chromium. We explain the effect by variations of the electronic structure in the alloy with concentration. Consequences of the strong concentration dependence of the interatomic interactions in Fe-Cr system are discussed.

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[2] L. Vitos, I. A. Abrikosov, and B. Johansson, Phys. Rev. Lett. **87**, 156401 (2001).
[3] P. Olsson, I. A. Abrikosov, L. Vitos, and J. Wallenius, J. Nucl. Mat. **321**, 84 (2003).
[4] P. Olsson, I. A. Abrikosov, and J. Wallenius, Phys. Rev. B **73**, 104416 (2006).

Equilibrium phase diagrams

M-N. de Noirfontaine, C. Girod Labianca, Pr. G. Inden

1. Basic Thermodynamics

• Definition and experimental determination of an equilibrium phase diagram
Temperature = f (time) curves, diffusion measurements, phase characterization methods…
• Thermodynamic study of phase diagrams and minimisation of the Gibbs free energy
From the Gibbs free energy variations of the phases, G(X,T), to the determination of the phase diagram (X: Composition, T: Temperature)
- Pure compounds: melting points (T_m) determinations
- Binary systems: liquidus and solidus lines determinations
Chemical potentials and common tangent construction

2. Introduction to "CALPHAD" formalism

CALPHAD = CALculation of PHase Diagrams
From experimental thermodynamic data to G(X,T) polynomial functions
• Thermodynamics models for solutions and compound phases → G(X,T)
- Stoichiometric compounds: G = G(T) polynomial functions
- Solution Models: G(X,T) polynomial functions and model parameters
Ideal mixing, non ideal mixing: regular and non regular models (Redlich-Kister equation),...
• Refinements of the model parameters based on selected experimental thermodynamic data
Experimental determination of thermodynamic quantities: calorimetric methods
G(X,T) evaluation by assessment technique → thermodynamic databases

3. Introduction to Thermo-Calc software. Demonstrations and examples

• Thermo-Calc software = CALPHAD formalism + Thermodynamic databases of G(X,T)
Calculation of phase equilibria by Gibbs energy minimisation process
• Demonstrations and examples: Two cases
1) First case: all the phases of the studied phase diagram are well described in the databases in all the range of temperature and composition
Examples: Calculations of the Cu-Ni and Fe-Cr phase diagrams
- Features of the experimental known phase diagram
- Description of the phases in the database. Models and values of the parameters
- Plotting the calculated phase diagram and the thermodynamic functions
- Comparisons of the experimental and the calculated phase diagrams
2) Second case: all the phases of the studied diagram are not or only partially described in the databases. Introduction to the assessment technique and discussion

Technical support

PC with Thermo-Calc software installed for the course


Thermo-Calc software AB, Stockholm, Sweden
Web site: www.thermocalc.com

Crystal plasticity from Dislocation Dynamics

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This presentation will overview the premise and the promise of Dislocation Dynamics (DD) as a method for direct calculation of plasticity and plastic strength of single crystals from the underlying motion of dislocation lines. First, a few aspects of dislocation physics most relevant for the DD method development will be discussed followed by a brief introduction of several key algorithmic and numerical aspects of the DD method. Then, specific examples of applications of the DD method will be given to illustrate the method's ability to capture the essential physics of collective dislocation motion. The primary focus will be on BCC metals where several key results have recently emerged from DD simulations. Finally, the method's applicability to simulations of irradiated metals and alloys will be discussed along with the associated method development issues.

Microstructural & mechanical properties of irradiated structural materials

S. J. Zinkle

This plenary lecture is naturally divided into two parts, since the mechanical property changes are driven by radiation-induced microstructural changes in materials. In ML1-1, the current understanding of defect production (point defects and extended defects) and associated microstructural changes in neutron-irradiated body centered cubic (BCC) and face centered cubic (FCC) metals are reviewed as function of irradiation flux, dose and temperature. A wide range of microstructural changes can be induced by irradiation depending on the materials and irradiation conditions, including various dislocation loops or stacking fault tetrahedra, changes in the network dislocation density, radiation-enhanced, induced, or –modified precipitation, and cavity formation. A summary of currently available experimental tools for examining the microstructure of irradiated materials will be given, with primary emphasis on transmission electron microscopy but other valuable techniques including positron annihilation spectroscopy, electrical resistivity, field ion microscopy/atom probe tomography, and X-ray and neutron diffraction spectroscopy will also be briefly reviewed. Fundamental differences in the defect production and accumulation in FCC and BCC crystal systems will be emphasized. The pronounced effect of irradiation at temperatures within specific regimes will be illustrated, such as above/below the temperature for long-range vacancy migration. Examples will be given for both pure metals and complex high-performance alloys. The existing information concerning the "classical" and emerging steel grades (e.g., 9Cr-1Mo or advanced 12Cr ferritic/martensitic steels such as HCM12A or T122) will be presented, and illustrated with exemplary results from the literature.

In ML1-2, which is focused on radiation-induced mechanical properties changes, an overview will be given regarding the effects of irradiation dose and temperature on the mechanical properties of FCC and BCC metals. Particular emphasis will be placed on the similarities and differences of neutron irradiation on the tensile properties of pure metals and complex alloys. The effects of test temperature and strain rate on the tensile properties before and after irradiation will also be summarized. A common feature in all metals irradiated at temperatures below ~0.3TM, where TM is the melting temperature, is an increase in tensile strength and a decrease in uniform tensile elongation. Possible microstructural causes of the decrease in uniform elongation (localization of plastic deformation) will be discussed, including dislocation channeling. The results from in-situ tensile straining of specimens containing a variety of defect clusters will be summarized, along with molecular dynamics modeling of dislocation interactions with defect clusters, in order to provide insight on possible physical mechanisms associated with flow localization. The increased strength associated with irradiation at low temperatures can produce large increases in the ductile to brittle transition temperature (DBTT) of BCC materials. In addition to hardening effects on fracture, irradiation can also induce changes in fracture mechanisms due to radiation induced solute segregation to grain boundaries or other features. The overall effect of irradiation on the deformation and fracture behavior of metals will be summarized using deformation mechanism maps and fracture mechanism maps. Areas where additional data are needed to support the development of accurate physics-based models of hardening and embrittlement will be discussed.

ML2

Radiation-Induced Solute Segregation and Precipitation in Alloys

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Radiation-induced segregation (RIS) of atoms in solid solution is an important phenomenon in commercial alloys used in nuclear reactors. For example, grain boundaries in neutron-irradiated austenitic stainless steels eventually become depleted of Cr and enriched in Ni, with the deleterious consequence of promoting susceptibility to stress-corrosion cracking. It is therefore not surprising that RIS is currently a lively topic of research in the nuclear materials community. RIS was first observed in the mid-seventies, and it was realized almost immediately that the coupled diffusion of solute atoms and vacancies and/or interstitials to point-defect sinks must play an important role in the process. Shortly after the first observations of RIS, the related phenomenon of radiation-induced precipitation (RIP) in under-saturated alloys was discovered. This was exemplified by the unexpected heterogeneous nucleation of precipitates at dislocation loops, as well as at grain boundaries and free surfaces. Radiation-induced homogeneous precipitation in the interior of defect-free grains of under-saturated Ni-Si alloys was also observed. In this talk the fundamental aspects of RIS and RIP will be reviewed, starting with their early history and ending with the current state of understanding. RIS and RIP can also affect mechanical behavior at ambient and elevated temperatures. These consequences of RIS and RIP will also be discussed.

Parametric dislocation dynamics and boundary element modeling of elastic interaction between dislocations and precipitates

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The formation of precipitates and the interaction with dislocations in metals are responsible for the degradation of the material strength subjected to high-energy neutron irradiations. Understanding the interaction between the dislocations and precipitates, and the subsequent degradation of the material strength are thus very important. In this seminar, a hybrid computer simulation method with the combination of the parametric dislocation dynamics (PDD) and the boundary element method (BEM) to investigate the dislocation-precipitate interaction problems is presented, which enables us to simulate the interaction between a flexible dislocation and precipitates with any geometrical shapes. The method is first applied to the simulation of the interaction between a dislocation and a copper precipitate in bcc-Fe. The results show a good consistency with the results of molecular dynamics (MD). Then, we investigated the effects of the diameter, spacing and elastic constant of a spherical precipitate on the interaction with a dislocation. Finally, an extension of the present method to incorporate the dislocation core effects will also be presented.

GL6/S6

The Computational Modeling of Alloys at the Atomic Scale : From Ab Initio and Thermodynamics to Radiation-Induced Heterogeneous Precipitation

A. Caro
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Lawrence Livermore National Laboratory, USA

This paper describes a strategy to simulate radiation damage in FeCr alloys wherein magnetism introduces an anomaly in the heat of formation of the solid solution. This has implications for the precipitation of excess chromium in the α′ phase in the presence of heterogeneities. These complexities pose many challenges for atomistic (empirical) methods.

To address such issues the authors have developed a modified many-body potential by rigorously fitting thermodynamic properties including free energy. Multi-million atom displacement Monte Carlo simulations in the transmutation ensemble, using the new potential, predict that thermodynamically grain boundaries, dislocations, and free surfaces are not preferential sites for α′ precipitation.

GL6

Multiscale computer simulations and predictive modeling of RPV embrittlement.

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Structural materials used for nuclear components such as reactor pressure vessels and core internals the light waters are subjected to high-energy neutron irradiation that cause radiation damage in the materials. The accumulation of the radiation damage results in mechanical property changes in the materials, and thus, the understanding of the degradation mechanisms of the materials under irradiation conditions and its application to accurate prediction of the material degradation are very important for the safe and long-term operation of the nuclear reactors.

In this lecture, multi-scale computer simulation approach will be presented as a very powerful tool to understand the materials degradation mechanism over very wide time and length scales. Neutron irradiation embrittlement of reactor pressure vessel (RPV) materials is considered as an example of the success of this approach, where simulations of 1) point defect production by displacement cascades, 2) interaction of the defects with other defects and solutes during diffusion process, 3) characteristics of the defect or solute clusters, 4) interactions of such clusters with moving dislocations, and finally 5) mechanical property changes are performed by combining several computational techniques such as molecular dynamics, kinetic Monte Carlo and dislocation dynamics. Experimental results obtained by three-dimensional atom probe, positron annihilation, transmission electron microscope, and mechanical property test techniques will also be presented to compare with the simulation results.

Finally, all the information obtained by computer simulations and experimental results is integrated to develop a predictive model of RPV embrittlement, and the most recent method developed in Japan will also be presented.

Presentation of the Toughness Module

S. Bugat

One of the major issue of the European Project PERFECT from the 6th Framework Program is to provide a numerical platform aiming at predicting irradiation effects on RPV steels and internals. Such a platform contains 4 so—called "end-products", all based on multiscale approaches, for the prediction of the irradiated microstructures and the subsequent changes on mechanical properties: RPV-2 and the ToughnessModule, dedicated to RPV steels, and INTERN-1 and IASCCModule, dedicated to internals. We will focus only on the first two end-products.

RPV-2 starts from the irradiation conditions (neutron spectrum, in—service temperature, chemical composition of the RPV steel, irradiation time) and produces both the irradiated microstructure (i.e. the distribution of irradiation defects clusters) and the subsequent increase of hardness at the microscopic level (bainitic lath considered as a single—crystal). It can be chained with the ToughnessModule, which aims to provide both the irradiated macroscopic behaviour of the RPV steel, starting from the behaviour at the microscopic level (output of RPV-2), and the subsequent decrease in fracture toughness.

For each operation, the ToughnessModule can use different "branches". Each branch provides the same output but uses different physical modellings to obtain it, from the simplest and fastest one, to the more complex and CPU consuming one. All branches were specified by the sub-project 3 – RPV Mechanics of PERFECT.

For instance, as a first step, the macroscopic stress—strain curve of the steel can be obtained either using some kinds of property—property correlations (the increase of yield stress between the irradiated state and the un-irradiated state is proportional to the increase of critical resolved shear stress at the bainitic lath level), or by means of full finite element computation of a tensile test on a representative volume element representing a typical bainitic aggregate.

In the same way, for the second step, the decrease of fracture toughness can be estimated either by using semi-analytical models as the Master Curve, where the shift of reference temperature T0 is proportional to the increase of yield stress, or by a 1T-CT finite element computation where the behaviour was identified previously in the first step, and where the failure probability is estimated by a local approach post-processor as for the Beremin model.

Although a full and complete first version of the ToughnessModule was already delivered within the PERFECT project, it is still under heavy development in order to incorporate the latest scientific developments made within the project. In particular, a further version of this module will provide a so-called "sub-modelling" module, where the failure probability of a 1T-CT specimen will be evaluated by a complex model which parameters are only the carbide distribution of the steel, the microscopic behaviour of the steel and the metallurgical morphology of the bainite. Such a fully predictive model should allow the identification of the fracture properties from metallurgical observations and not from dedicated mechanical tests, which can be very interesting in particular for surveillance programs.

Kinetic MonteCarlo simulations of radiation damage in structural materials

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The kinetic MonteCarlo (KMC) method is a stochastic method intended to simulate the time evolution of some process. The treated system is advanced through time in an ordinary stochastic manner but with a timestep rigorously associated to each action. It is especially useful in studies of irradiation driven phenomena due to its power and flexibility. Although it was first developed in order to treat the diffusion of vacancices in a crystal lattice it has hence been developed in order to treat a vast range of phenomena. KMC is one of the few methods available to a nuclear scientist that can treat, on an atomistic level, spatial and temporal scales comparable to those in microstructural experiments.
This seminar will introduce you to the fundamentals of the kinetic MonteCarlo method, starting from the physical motivations and justifications and working through the mathematical formalisms towards a comprehensive understanding. Different KMC flavours will be discussed as well as their ranges of applicability. Novel schemes, such as parallelisation and action filtering will be treated. Finally, we will discuss some practical applications with implications for structural materials of nuclear reactor systems.

PRS 3&4

Electronic structure calculations in iron with defects (formation and migration energies) and/or gases (interaction vacancy – helium atoms)

G. Lucas, C.C. Fu

Introduction *(Lucas)*

Quantum mechanics => Schrödinger equation
Approximation of Born-Oppenheimer
Density Functional Theory (DFT)
- Origin and impact (Nobel Kohn 1998)
- The theorems of Hohenberg and Kohn
- The equations of Kohn et Sham
- The approximations for the exchange-correlation energy (LDA, GGA,...)
- Pseudopotentials and basis functions
- Limitations of DFT
- Examples and applications

Discovering one DFT code : Siesta (*Fu)*

Descirption of the principles of the method, key choices and parameters in an input file => practical concepts (k-grid, electronic convergence and structural optimization...)

Example of application (1): point defects in bcc iron *(Fu)*

- Stability of different structural-magnetic phases of iron
- Determination of relative stabilities of different self-interstitial configurations (<110> vs. <111>)
- Effect of magnetism
- Comparison of DFT and experimental results
- Using the calculated energies as input data in a “Rate Theory” code to explore the consequences of DFT results (optional, depending on time availability)

Example of application (2): defects in SiC *(Lucas)*

- Band structure of SiC
- Determination of the electronic band gap (semi-conductor) and comparison with experience (“Band Gap Problem”)
- Estimate the formation energy of a self-interstitial atom:
- Show the covalent nature of the bonds (density plot)
- Calculate the migration energy barrier by using a method of saddle point searching (depending on time availability)

GL4

Neutrons and radiation damage in structural materials

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In a nuclear reactor, neutrons do not only cause fission of actinides, they also interact with nuclei in the structural materials of the system. All these interactions cause damage in one or the other way. The most common mode of damage is a displacement of the constituent atoms of the structural material from their equilibrium lattice position, leading to formation of vacancies and interstitials. In fast neutron reactors, we will also have a significant rate of nuclear transmutations taking place, leading to formation of elements that tend to degrade mechanical properties and shorten the service time of both fuel and reactor vessel. When designing Generation IV nuclear systems, it is therefore important to fully understand such reactions in order to reduce the probability for failure. One would of course also like to develop materials that are more transparent to interactions with neutrons than the ones present in use.
After this lecture, you will be able to explain how the following nuclear reactions leads to radiation damage in steels that may be used for fuel clad or pressure vessels:

- Scattering of neutrons
- Capture of neutrons
- Neutron induced production of helium
- Neutron induced production of hydrogen

You will also be able to identify nuclear systems where the rate of damage due to scattering is lower than in others. Finally, you will be able to select structural materials that permit to reduce the rate of neutron capture and helium production.

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SiC as a material for application in generation IV systems: electronic, structural and mechanical properties

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There are many challenges to overcome before Generation IV fission reactors become commercially viable. Some of the most important challenges in both thermal [Very-High- Temperature Reactor (VHTR), Supercritical-Water-Cooled Reactor (SCWR), and Molten Salt Reactor (MSR)] and fast reactors [Gas-Cooled Fast Reactor (GFR), Sodium-Cooled Fast Reactor (SFR), and Lead-Cooled Fast Reactor (LFR] involve materials issues. They include the material employed in the reactor walls, the cladding material for the fissile nuclear fuel,and the material used for retaining the fission products. In addition to long term resistance to irradiation, the materials used in a nuclear reactor must have excellent mechanical and corrosion properties in order to tolerate the thermal shocks as well as the high temperature and severe corrosive environments that they will encounter during operation. One of the materials that has long been considered for this purpose is SiC, a material that is used both for its ceramic characteristics, as well as its wide bandgap semiconducting properties. In this talk, we discuss recent results on the mechanical and fracture properties of SiC and how the various defects affect the electronic properties of this high-temperature semiconductor.

Chemical compatibility of SiC composite structures with GFR helium at high temperatures – bibliographic review

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Silicon carbide ceramic matrix composites are promising candidate materials for structural components in the core of a Gas-cooled Fast Reactor (GFR) because of their high strength, adequate thermal conductivity and potential irradiation resistance at elevated temperatures and under high fluencies. Chemical compatibility with the typical reactor environment is a key point of the feasibility demonstration in normal service conditions as well as in any incident situation.

The gas composition, related to the core design, is not accurately known in this early research stage. The reactor coolant will inevitably be polluted by air ingresses during maintenance and refuelling operations as well as by slow out-gassing out of insulation and fuel materials. These impurities are ready to interact with hot in-core materials producing a specific atmosphere with low concentrations of oxygen, nitrogen, water vapour, possibly carbon oxide, hydrogen, methane… In any case, low oxygen potentials are expected and the high temperature behaviour of SiC composites in weakly oxidizing conditions has to be demonstrated. A literature review shows that:

- *massive silicon carbide* forms a dense surface silica layer when exposed to oxidizing atmosphere, such as air, and further oxidation is strongly reduced. Because of this passivation SiC exhibits excellent resistance at high temperature. However in inert or reducing atmosphere, oxygen supply is not sufficient for the protective silica film to be formed or SiO_2 is unstable. The gaseous lower oxide SiO is then produced and the ceramic decomposes by active oxidation. Such corrosion can significantly affect the mechanical strength by introducing flaws or reducing the load bearing cross section.
- *SiC composites* contain an interface material, usually made of graphitic carbon or hexagonal BN, that controls the friction and bonding between the fibres and the matrix. When gasses have an access (through flaws, porosity…), the interface can be oxidised. The oxidation products of graphite are gasses; the oxidation products of BN in water vapour are also volatile. The corrosion rate of the interface depends on the oxygen potential and the lower the oxidation potential, the slower the corrosion. However slow in weakly oxidizing conditions, the corrosion should continuously remove the interface material; the result could be a weakened composite due to the loss of contact between fibres and matrix.

Preliminary to the investigation of the long term corrosion resistance of such a complex material as SiC composite, it is relevant to study the individual behaviour of each component: matrix, fibres, interface. Two main corrosion processes may occur at elevated temperatures in the GFR helium which is polluted by traces of oxidizing and possibly reactive or reducing gasses: at low oxygen potential, the volatilisation of silicon carbide, fibres and matrix, with release of the volatile oxide SiO and the recession of the interface due to the formation of gaseous oxidation products. Both processes may strongly affect the mechanical resistance of the composite.

The Effects of Irradiation Damage in Structural Ceramics

L.L. Snead
Oak Ridge National Laboratory

Ceramic materials have been used as structural components in nuclear reactors since the very beginning of nuclear power. However, their application has been limited by both fundamental material performance limits (such as lack of tensile strength and fracture toughness) and their response to fast neutron damage (dimensional instability and loss of strength.) With the relatively recent development of fiber composites the intrinsic performance limits of ceramics have been significantly enhanced, yielding not only much tougher ceramics, but materials which fails in a more predictable manner, easing issues with regard to designing with brittle materials.

This paper will discuss in some detail the development path for silicon carbide composite, the most widely studied nuclear "structural ceramic." Particular emphasis will be first on the irradiation effects in silicon carbide from both a microstructural and thermomechanical response viewpoint. This system will be contrasted with other nuclear ceramics, such as graphite, beryllium oxide, and aluminum nitride, in an effort to describe where fundamental limitation exist and where additional development could allow significant improvement of alternative ceramics. Following this rather fundamental discussion of the ceramics irradiation effects, the interrelation of the changing properties of the composite constituents(fiber, matrix, and interphase), which has been shown to be the key to composite performance will be presented.

GL7

Fundamentals of Liquids

J-P. Hansen
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I will present an introduction to a Statistical Mechanics description of the liquid state of matter focussing on “simple” molecular, ionic and metallic liquids. A molecular level description is challenging, because liquids combine structural disorder and strong interatomic coupling (high density).

Short-range order (local molecular packing) controls the thermodynamic properties of liquids within a generalized van der Waals description of cohesion (equation-of-state, free and internal energy, …) as well as phase diagrams (condensation, demixing, freezing) while fluctuations determine the compressibility, heat capacity and dielectric permittivity.

Moving to dynamics, I will show the link between macroscopic transport (diffusion, thermal and electric conductivity, viscosity) and time-dependent correlation functions; the latter also determine quasi-elastic light and neutron scattering cross sections. Static and dynamic correlation functions can be extracted from molecular simulation methods, like Molecular Dynamics and Monte Carlo.

In the last part of my presentation I will briefly address some important specific aspects, including inhomogeneous liquids and interfaces, ionic liquids (molten salts), metallic liquids, and liquids under extreme conditions (supercritical behaviour).

GL9

Fundamentals of Interfaces

P. Wynblatt

The aim of this lecture is to provide an overview of fundamental notions on surfaces and interfaces. This will begin with an introduction to the thermodynamics of interfaces, using the Gibbsian approach, which will cover the concepts of the Gibbs Dividing Surface and of interfacial excess quantities. Particular attention will be paid to interfacial adsorption and/or segregation phenomena, through the use of Gibbs and McLean isotherms. This will be followed by an introduction to grain boundary (GB) structure, including simple twist and tilt GBs as well as a description of general GBs by means of the five macroscopic degrees of freedom of GB character. GB segregation will be discussed together with the transition from segregation to wetting of the GB by a second phase. Anisotropy of the interfacial properties will be emphasized throughout. The lecture will end with an introduction to diffusion in solids, in which Fick's law, vacancy diffusion and the Arrhenius relations for volume and GB diffusion will be discussed.

GL8

Wetting

D. Chatain, V. Ghetta

The first part of this lecture will use the background provided by the previous lecture on Fundamentals of Interfaces to introduce the fundamental aspects of wetting, including contact angle, and partial and complete wetting at surfaces and interfaces such as grain boundaries. The concepts of thermodynamic adhesion and wetting hysteresis will be explained.
In a second part, emphasis will be placed on real wetting by liquid metals. Various types of wetting (reactive and non-reactive) will be introduced, and the impact of surface heterogeneity on wetting in practical situations will be illustrated. The trends in wetting in metal/oxide and oxide/metal systems will be summarized. Finally, the difficulties encountered in wetting studies at surfaces and grain boundaries, as well as issues of special interest to generation-IV systems will be discussed.

Thermophysical properties of liquid metals and alloys, an experimental approach

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Over the past years an increasing demand for thermophysical data of liquid metals has been noticed. Properties of matter at high temperatures are useful for high-temperature technologies such as aerospace, nuclear energy and the establishment of temperature reference points, as well as for modelling, i.e., the mathematical modelling of casting processes, or to obtain phase diagrams.

Only few techniques have been established to perform measurements on physical properties of metals and alloys up to temperatures in the liquid state. One of these techniques is the so-called ohmic pulse-heating, which has successfully been used by different institutions around the world to obtain temperature dependent thermophysical data. At the Institute of Experimental Physics, Graz University of Technology, Austria, a constantly improved pulse-heating setup has been used for more than two decades now to determine thermophysical properties of metals and alloys in the solid and the liquid states.

In the list of thermophysical properties, some properties are of greater importance for use in industrial applications, while others are of more scientific interest for different applications. The properties which will be discussed here are heat of fusion and heat capacity, electrical resistivity, thermal expansion, density, thermal conductivity, thermal diffusivity, and hemispherical emittance as a function of temperature. How to obtain critical pressures within pulse heating experiments also will be discussed.

To complete the set of thermophysical properties of liquid metals, viscosity and surface tension measurements performed in other laboratories with levitation techniques also will be presented.

Liquid sensors : Principle and measurements

J. Fouletier, V. Ghetta

The use of the proposed coolants for the different generation IV systems, whatever alkali metals (sodium, etc.) for SFR, Heavy Liquid Metals (Lead, Lead-Bismuth eutectic and possibly other lead alloys) for Spallation targets, ADS, or LFR molten salts (of type $LiF\text{-}UF_4\text{-}ThF_4$.etc.) for MSBR concept, requires the control of some species in the liquid phase, depending on the reactor type. In any case, this control is essential in order to monitor corrosion and/or mechanical resistance of structure materials at long term, and it implies the measurement of chemical activities in liquids.

The aim of this lecture is to give basic knowledge on thermodynamic properties of liquid mixtures, on activity (definition, reference state, role in corrosion processes) and on principles of electrochemical measurements for activity monitoring. Then, the state of the art and the ongoing research for each type of needed sensors will be detailed, with their possibilities and limitations.

ML5

Influence of Liquid Sodium on mechanical properties of steels, refractory alloys and ceramics

H.U. Borgstedt, FZK, Germany

Part 1: Corrosion and Reactions with Impurities Dissolved in Sodium

The first part of this plenary lecture deals with the corrosion processes that influence the material hehaviour. Corrosion causes mass losses and selective leaching of alloying metals, and intercrystalline effects can occur due to the corrosion reactions. Sodium and solid materials are able to exchange interstitial components as non-metallic elements the most important of which are carbon and nitrogen. Some alloys pick up oxygen from sodium even at concentrations of 5 mg/g in the liquid phase. Internal oxidation is the corrosion process in this case. Hardened or even brittle surface layers are produced. This experience is based on the work for the SNR 300 reactor in cooperation with Belgium, the Netherlands and German Industries. A project with the Kalpakkam Centre in India brought further experience into the knowledge on the exchange of non-metals.

Part 2: Creep Rupture and Low Cycle Fatigue of Reactor Materials in Liquid Sodium

Since the corrosion reactions may influence the long term mechanical behaviour of the structural materials, studies of the creep-rupture properties of steel 304 and 316 up to 10000 hours under load and in contact with flowing liquid metal were performed for the European Fast breeder project in cooperation between laboratories in France, the United Kingdom and Germany.

The low cycle fatigue behaviour of such steels was also studied in flowing sodium. The equipment for such experiments ˆ encapsulated fatigue specimens ˆ had to be developed. The influence of flowing sodium on the low cycle fatigue behaviour of the two steels is not significant. The influence of corrosion and exchange of interstitials on the mechanical behaviour is discussed. The results of these studies have been discussed with Japanese scientists. Further mechanical tests in sodium loops were performed in the Kalpakkam Centre.

TL5

Chemistry control in large installations: requirements, purification strategies, system design

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Liquid sodium is extensively used as a coolant for Fast Neutron Reactors because of its very attractive thermal, hydraulic and neutronic properties as well as for its low cost. However, sodium is characterized by its high chemical activity with regards to several elements or compounds, and to oxygen in particular. Oxygen is introduced in the various parts of the reactor, particularly during the start-up operations and latter during handling operations, even if the ingress is always limited, thanks to some very efficient procedures In the primary vessel, oxygen contributes to the corrosion phenomena and therefore to some general mass transfer of activated products from core to the coldest parts of the reactor, ie the heat exchangers; dissolution of main constitutive elements of the steel is also a main contribution to the mass transfer, even if this dissolution is much lower than with other coolants as lead alloys. The main consequence of this mass transfer is the following one : contamination of internals and components and therefore necessity to decontaminate the structures in order to reach an acceptable dosimetry in case of handling and repair operations. Some very low source of tritium is also produced in the control rods and released in the sodium ; it is also produced by ternary fissions. In case of pin rupture some fissile material and fission products like caesium can be released in liquid sodium. Many countries have chosen to apply a policy of maintaining the primary sodium at its “maximal” purity, in fact to maintain the oxygen concentration lower than 3 wppm, in normal operation.

The intermediate loops, used to transfer the nuclear heat from the primary vessel to the Steam Generators Units, can also be polluted by initial impurities like oxygen and hydrogen, present on the structural material surface as adsorbed oxygen and moisture, by products induced by the sodium-water incidental interaction and also by a continuous source of hydrogen, produced by aqueous corrosion, which permeates from water side to the sodium of the intermediate loops. The detection of a water ingress is based on the hydrogen detection; therefore, it is necessary to maintain in normal operation a very low hydrogen concentration, for a very efficient and fast detection of sodium-water interaction, namely below 0.1 wppm and often lower.

“Primary” or “intermediate” sodium must be purified, in order to reach the quality specifications, thanks to the Purification System, usually based on the use of cold trap, thanks to the oxygen and hydrogen solubilities in sodium, which are close to zero, near the sodium melting point. Several purification strategies and cold traps have been developed in the past for various applications. In this lecture we will recall the purification requirements, describe the purification systems and more particularly cold traps, design based on crystallization mechanisms and kinetics. An overview of the existing purification systems used in the world in the existing reactors but also foreseen for the on-going projects will be performed.

Other purification technologies like O gettering will be also investigated.

For the future SFR, Supercritical CO_2 Brayton Cycle could be a promising option to enhance the competitiveness of the future Sodium Fast Reactors. Nevertheless an interaction of sodium with supercritical-carbon dioxide can occur in case of CO_2.ingress. The purification by adapted means to eliminate potential particles, cover gas purification, will be also adressed…

GL10

Liquid metal embrittlement

D. Gorse

Structural Materials for Fusion Power Plants
Part I: Radiation Effects and Major Issues

J- L. Boutard EDFA - Close Unit Support GARCHING (D)

The decision of constructing ITER has opened the perspective for a fusion reactor demonstrating the feasibility of the thermo-nuclear fusion energy production. The selected D-T fusion reaction releases one 14.03 MeV neutron and one 3.56 MeV helium. Elements of design of the main in-vessel components of a fusion power plant, i.e. tritium-breeding blanket, divertor and first wall, will be presented. The structural materials for these components will have to withstand high doses of ~100 dpa and production of transmutation elements such as He (~10 appmHe/dpa) and H (~45 appmH/dpa) induced by the 14.03 MeV neutrons. In addition the divertor will have to undergo high heat fluxes ~10 MW/m^2.

The irradiation by the 14.03 MeV neutrons will affect the materials at the atomic scale: (i) the crystalline structure is locally destroyed by displacement cascades, (ii) the chemical bonds are strained by He and H transmutation products, and (iii) radiation induces microstructure changes controlled by point defects and impurities diffusion. The basis for the selection of structural materials which will have to be radiation resistant under such condition will be reviewed.

For Tritium (T)–Breeding Blankets, Reduced Activation (RA) 9 % Cr ferritic martensitic steels for temperatures up to ~550 ^{0}C and Oxide Dispersion Strengthened (ODS) ferritic steels up to ~750 ^{0}C have been selected on the basis of their well known metallurgy and high resistance to neutron irradiation in fast reactors. SiC_f-SiC composites envisaged as prime candidate for high operating temperatures have been selected on the basis of the high stability of the newly developed and nearly stoichiometric β-SiC fibres. For the divertor, high thermal conductivity Cu-alloys or W-alloys are to be used to withstand the high heat flux of ~10 MW/m^2.

The most significant experimental results about point defect & He accumulation and phase stability, which control the hardening and embrittlement of ferritic martensitic steels, will be presented. The radiation stability of Cu-alloys, either precipitation hardened such as Cu-Cr-Zr or Oxide Dispersion Strengthened such as Cu Al_2O_3 will be summarised. The issues concerning the initial fracture toughness and in–service phase stability of the W-alloys will be underlined. In the absence of an intense 14.03 MeV neutron source various irradiation techniques are used: (i) alpha particles implantation, (ii) irradiation in fast neutron spectrum or mixed spallation-neutron spectrum, (iii) ion beam irradiation in dual or triple beam configuration, to assess the radiation effects on the in-service properties in the future fusion reactors. The main issues concerning the relevance of these techniques to simulate 14.03 MeV neutron radiation effects will be discussed.

Most of the metallic alloys irradiated at low temperatures show localisation of the plastic deformation in the so-called clear channels when tested out of flux in hot cells. Recent in-pile tensile tests will be presented questioning such behaviour under irradiation.

Qualification of these materials should be carried out in the future International Fusion Material Irradiation Facility (IFMIF) based on D-Li reaction producing a neutron spectrum very similar to the D-T fusion one. The main characteristics of IFMIF and a final overall view of all the irradiation techniques used to simulate radiation effects under fusion reactor conditions will be presented in term of dpa and He production.

Part II: Multi-scale Modelling Radiation Effects

J- L. Boutard EDFA - Close Unit Support GARCHING (D)

The European fusion program on radiation effect modelling has been launched in 2002 to study and correlate the radiation effects under the various spectra used to simulate the D-T fusion neutron spectrum. The main objective is to develop modelling tools to study radiation effects in the reference martensitic steel EUROFER under fusion reactor relevant conditions. Such a modelling is multi-scale in nature. The emphasis has been put on the physics of radiation-induced processes and its experimental validation at every space and time scale. The effort has been devoted to (i) ab-initio determination of the Fe-Cr system cohesion and of the energetics of point defects, He and carbon in α-Fe and Fe-Cr model alloys, (ii) multi-scale modelling of kinetics of radiation effects controlled by diffusion (iii) development of inter-atomic potentials for Molecular Dynamics (MD) simulation of displacement cascades and dislocation dynamics.

The presentation will give a brief review of the various theoretical tools used in multi-scale modelling radiation effects: (i)ab-initio calculation based on the Density Functional Theory, (ii) Molecular Dynamics for fast kinetics, (iii) Monte Carlo methods and Mean Field Theory method such as Rate Theory for diffusion controlled kinetics and (iv) Dislocation Dynamics for the collective behaviour of dislocations.

Recent ab-initio calculations concerning the formation energies of Self Interstitial Atom (SIA) in bcc transition metals showed the essential role of magnetism in α-Fe. Formation energies and diffusion pathways of small vacancy and interstitial clusters ($n<4$) computed in the DFT approximation were used to reproduce via Kinetic Monte Carlo the radiation damage recovery stages in α-Fe. Ab-initio energetics of He and point defects in the system Fe-He-C enabled reproducing He-desorption kinetics via Monte Carlo and Rate Theory. DFT calculations of various configurations of the Fe-Cr system in the Fe-rich range allow understanding the role of magnetism in the behaviour of the system. Exchange Monte Carlo method based on Cluster Expansion fitted on these ab-initio results gives new insight into the phase diagram of the Fe-Cr system and allow reproducing the ordering and clustering tendency of Cr atoms below and above ~9% Cr respectively.

Ab initio data can also be used to fit the empirical potentials required for Molecular Dynamics simulations. The newly developed potentials, based on different assumptions but all reproducing the correct energetics of SIAs in α-Fe, result in reducing considerably the so far unacceptable scatter of Frenkel pairs production obtained in the Molecular Dynamics (MD) simulation of displacement cascades. Semi-empirical potentials were developed to reproduce the negative mixing enthalpy of the Fe-Cr in the low Cr content domain of interest, Cr point defect interaction and primary damage using MD simulations.

The program is now focused on (i) developing reference kinetic tools to predict the Fe-Cr system phase transformation kinetics able to take into account explicitly the magnetism and effect of carbon, under thermal ageing and irradiation (ii) predicting, at the atomic scale, the screw dislocation core structure and glide mechanisms (iii) parameterising Discrete Dislocation Dynamics code to describe the collective behaviour of dislocations at the meso-scale, and (iv) carrying out validation experiments using extensively the multi-beam facility JANNUS. JANNUS will allow irradiating with double (dpa, He) or triple (dpa, He, H) beams and characterizing (TEM, AP-FIM, nano-indentation) volumes of the same order as the ones that can be numerically simulated.

The development of physically based modelling tools to study and reliably predict radiation effects in the Fe-x%Cr-C ferritic model steels is now a realistic medium term objective.

Operation of high power liquid metal spallation targets: A challenge for structural materials

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High power liquid metal spallation targets produce intense fluxes of neutrons which can be used either for neutron scattering experiments or to drive subcritical nuclear reactors (the so called ADS: Accelerator Driven Systems) dedicated to the transmutation of radioactive wastes. Several projects aiming at developping such neutron sources are currently underway in different countries worldwide. In the present seminar, we will focus primarily on one example, the MEGAPIE target, a 1 MW liquid Pb-Bi target which was successfully irradiated at PSI from August to December 2006, a first-of-its-kind experiment. However, we will also mention the SNS (the US Spallation Neutron Source, located at ORNL) which is in the startup phase for full power operation.

After having briefly described the proton accelerator system at PSI and the characteristics of MEGAPIE, we will present the reasons for the choice of the main structural materials of the target. We then show that these structural materials and in particular the material of the “beam window”, are subjected to very severe operating conditions and we review the different causes of damage, possibly acting synergistically: corrosion/erosion by the liquid metal, irradiation embrittlement by energetic protons and neutrons, Liquid Metal Embrittlement (LME)/Liquid Metal Accelerated Damage (LMAD). Moreover, in the case of the pulsed source SNS, whereas MEGAPIE is a continuous one, a specific phenomenon may occur : cavitation erosion by bubble collapse on the target walls. We will then present and discuss the results of a number of experiments designed such as to address the materials issues.

In the final part of this presentation, a brief account of the irradiation phase of MEGAPIE will be given, followed by a description of the planned Post Irradiation Experiments (PIE) which will be a unique opportunity for obtaining data on materials behaviour under the prototypic operating conditions of liquid metal spallation sources.

Research and Development of Oxide Dispersion Strengthened Ferritic Steels for Sodium Cooled Fast Breeder Reactor Fuels

M. Inoue, T. Kaito and S. Ohtsuka

Oxide dispersion strengthened (ODS) ferritic steels is eligible for fuel pin cladding tubes to endure heavy displacement damages up to 250 dpa at high temperatures up to 973 K in commercialized sodium cooled fast breeder reactor (SFR) cores. Ferritic steel (bcc) is essential to prevent from void swelling, which emerges in austenitic steel (fcc) obviously over 100 dpa. Dispersion hardening is indispensable for higher temperatures than 923 K, where precipitation hardening in ferritic-martensitic steels loses its ability. For ODS steels, powder metallurgy process including mechanical alloying and hot consolidation produces highly stable and very fine oxide dispersoids in matrix, and provides excellent dispersion hardening.

Japan Atomic Energy Agency (JAEA) has been developing ODS steels since 1987. We focused mainly on 11 to 13 mass% Cr ODS (12Cr-ODS) steels in the former decade, and have gradually shifted to 9 masss% Cr ODS (9Cr-ODS) steels in the latter. In 1999, we manufactured dozens of cladding tubes for both 9Cr- and 12Cr-ODS steels which meet targeted creep rupture strength equal to 120 MPa for 10,000 hours at 973 K under internal pressure. It is noteworthy that the target strength is comparable with austenitic stainless steel such as the modified SUS316.

During the Feasibility Study on Commercialized Fast Reactor Cycle Systems from 1999 to 2005, we have selected 9Cr-ODS steel as the primary and 12Cr-ODS steel as the secondary. Chemical composition of the 9Cr-ODS steel is defied as Fe-0.13C-9Cr-2W-0.2Ti-0.35Y_2O_3 in mass%, and final heat treatment condition is normalizing at 1,323 K for 1 hour followed by tempering at 1,073 K for 1 hour with air cooling. Ti addition with Y_2O_3 enables to uniformly disperse a few to several nanometer size complex oxides and enhances dispersion hardening effect. Alloying tungsten up to 2 mass% offers solution hardening with little detrimental laves phase precipitations. As internal pressure in a fuel pin increases with burnup due to noble gas accumulation, cladding tubes should be stronger against hoop stress than axial stress. Cold-working process in tube manufacturing tends to result in anisotropic grain growth, and then grain boundary sliding easily occurs and contributes to deform under hoop stress in low strain rate regime. However, alpha to gamma phase transformation for 9Cr-ODS and recrystallization for 12Cr-ODS steels can modify grain morphology and improve creep rupture strength. In addition, appropriately combining intermediate or final heat treatment temperatures with cooling rates can either soften or harden matrix in the cold-rolling process.

The tubes have been extensively tested for mechanical properties in air and stagnant sodium environments to establish the Material Strength Standard (MSS) for fuel pin mechanical design. Also, hundreds of specimens have been irradiation-tested in the experimental fast reactor JOYO to investigate irradiation effect on dimensional and mechanical properties. In-pile creep rupture tests using pressurized tube specimens have been also carried out by the Material Testing Rig with Temperature Control (MARICO) in the JOYO. Post-irradiation examinations for tensile specimens after exposure up to 15 dpa revealed that, for both 9Cr- and 12Cr-ODS steels, no irradiation effect on uniform elongation is observed and that there are slight increases in proof and ultimate tensile strengths.

Both 9Cr- and 12Cr-ODS steel tubes with vibro-packed mixed oxide (MOX) fuel particles were assembled into fuel pins, and have been irradiated since 2003 under a collaborative program between JAEA and Research Institute of Atomic Reactors in the BOR-60 in Russia; peak dose is targeted at 75 dpa and maximum temperature at 973 K. Pressurized resistance welding technology has been applied to join the tubes and end plugs. We will irradiate six fuel pins, which are clad with the 9Cr-ODS steel and loaded with annular MOX fuel pellets, in the JOYO from 2008; target dose is 210 dpa with peak burnup: 180 GWd/t by 2015.

In the Fast reactor Cycle Technology development (FaCT) project, we concentrate on the 9Cr-ODS steel, develop large scale tube manufacturing technology for mass production, and prove the MSS by a series of irradiation tests.

GL11

The TMSR Concept: Molten Salt Reactors in the Thorium Fuel Cycle

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We start with a brief historical introduction of the concept of Molten Salt Reactor (MSR). After a global description of MSRs (core design, liquid fuel salt, reprocessing) and of the Thorium fuel cycle, we will present some parametric studies of the neutronic behavior of these Thorium Molten Salt Reactors (TMSR) in terms of moderation ratio, fuel salt composition, reprocessing design and efficiency… We will more precisely analyze some key points of a reactor's operation, which are the fuel evolution, the waste production, as well as the safety coefficients, and more specifically the reprocessing scheme and its influence on the core operation. Finally, through worldwide or regional deployment scenarios of TMSRs, we will demonstrate how the Thorium cycle could be launch, while managing the waste currently produced.

Physical and chemical properties of molten salts

J-C. Poignet and J. Fouletier

Molten salts can be suitable to handling very reactive elements, for various processes such as preparation, partitioning, chemical or electrochemical reprocessing : for example, Na, Li, Ca, Al, F_2 are prepared by molten salts electrolysis on the industrial scale. Furthermore, reactions in such highly concentrated ionic media are very fast.

General features concerning properties of molten salts (temperature domains of possible use, thermal, chemical or electrochemical stability) are given and commented.

Focusing on molten halides, which are most appropriate to various applications in nuclear energy, a survey of physical parameters such as density, vapour pressure, transport properties (diffusion, viscosity, electrical conductivity), is given.

Chemical properties (acido-basicity, particular role of oxide ions and of water, complexation) are commented and methods for preparation and purification of molten halides are briefly described. Electrochemical properties (standard potential scales) are presented. Finally, electrochemical methods usable in molten salts for analysis or processing are briefly described.

ML6

Combined effect of molten fluoride salt and irradiation on Ni-based alloys

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Fluid fuel (in form of molten fluoride salts) is considered as a promising non-traditional fuel in several projects of the Generation IV Nuclear Systems (G-IV), e.g. transmutors and thorium reactors. Molten salts (MS) are candidate coolants for high temperature reactors to produce electricity and process heat for hydrogen production. Thus the MS has to be compatible with piping and heat exchanger materials. A challenge for using molten fluoride salts is their corrosive nature. R&D of construction materials compatible with MS at high temperature is the key problem of the G-IV projects.
Ni-Mo alloy (Hastelloy N) was used in MS experiment in Oak Ridge many decades ago. This experience was promising but it is not enough for designing of constructions and use of the proposed G-IV reactors for a long time. Some investigation of role of alloying additions on the Ni-based alloy corrosion in convective MS loop were performed later but combined effect of MS and irradiation on Ni-based alloys was never investigated before experiments performed in National Science Center “Kharkiv Institute of Physics&Technology”. The lecture is dedicated to the experiment methodology and results obtained.
To perform the experiment, Electron Irradiation Test Facility (EITF) was designed, constructed and used with a linear electron accelerator of 10 MeV energy. The electron irradiation was chosen for the following reason. Since the corrosion is controlled by chemical reactions and the reaction rate is rather sensitive to the local energy deposition due to irradiation, the electron irradiation which provides a variety of deposited energy values in surface layers of the tested samples is an efficient instrument for imitation of the reactor irradiation. In parallel, the electron irradiation impacts diffusion and phase transformations in bulk and, especially, within the grain boundaries.
Two Ni based alloys differing in composition by dopants Nb (0. 5%) and Y (0. 05%) were tested using EITF. Both alloys possess acceptable corrosion resistance but the corrosion rate under irradiation is some orders in magnitude higher than that without irradiation. Investigation of the role of Nb and Y dopants in Ni-Mo alloys on the corrosion under electron irradiation at 650° C shows that they change both the character of the corrosion and the corrosion rate sensitivity to the energy deposited. Carbon-carbon composites were tested as well. They showed rather high corrosion and irradiation resistance in MS.

To conclude, the R&D to be conducted, in collaboration between nuclear physicists, condense matter physicists and metallurgists, will be discussed, pointing out the key issues to solve in order to demonstrate the feasibility of G-IV projects.

GL12

Specific features of particule/matter interaction for accelerator-driven sub-critical reactors

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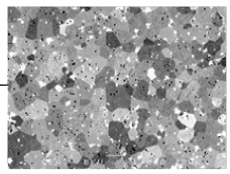
High-intensity beams of high-energy protons bombarding a heavy metal target can produce through spallation reactions intense neutrons fluxes. The lecture will first describe the possible applications of these intense neutron fluxes with emphasis on accelerator-driven sub-critical reactors that are envisaged for the transmutation of nuclear waste. The main existing neutron sources and projects of ADS will be briefly presented.

We will then describe the mechanism and characteristics of the different types of nuclear reactions that occurs in ADS: from high-energy (around 1 GeV) reactions encountered in the target and window to secondary reactions at much lower energies taking place in the structural materials. The specific implications for radioactivity production and material damage will be discussed. The general features of the simulation tools used to design ADS will be presented.

In the next part, we will study in details the modelling of spallation reactions. The basic hypotheses used to describe the reaction mechanism will be recalled and the recent developments discussed. In particular, it will be shown that the large amount of high-quality data collected during the last 10 years has permitted to improve significantly our understanding of the reaction mechanism and develop models with a better predictive power. The precision with which each quantity important for applications, as radioactivity, gas production or atom displacements, can now be predicted will be discussed. Remaining deficiencies and limitations will be addressed and perspectives for further improvements and extensions of the models will be presented.

As an example of recent progress made in experimental techniques, a separate lecture will be devoted to the detailed description and results of the experiments done at GSI, Darmstadt, using the reversed kinematics method. These experiments have allowed determining the complete isotopic yields and recoil velocities of the spallation residues in lead and iron, which are major components of respectively the target and the window. The impact of these results on applications will be discussed.



1

On Design Fuel with Small Swelling

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PACS: 61.72.Ww, 61.43.Er, 65.40.-b
Key words: nuclear fuel, swelling, vacancy, cluster, designing, fractal microstructure.

In developing the methods for designing reactor materials as to nuclear fuel, the task for microscopic-structure suppressing the processes of its swelling on the macroscopic defects (clusters, precipitations, vesicles, pores, cracks) is formulated here.

For controlling the defective structure of fuel during irradiation, it is offered to choose such the eutectic composition of that and develop its glassing technology so there would be the steady-state fractal tetrahedral clusters of dense part of amorphous phase in the initial random nuclear-fuel matrix.

In this connection, a search of threefold eutectic alloy in the system UO_2–UC–USi can appear a perspective direction for designing the fuel with small swelling factor. Such the fuel will have high volumetric density of equilibrium vacancy microdefects that effectively absorb solid and gaseous fission products and reduce the swelling.

The Effect of Ln(III)/An(III) Separation on Feasibility of TRU Recycling

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Keywords: lanthanide actinide separation, transuranium elements recycle

One of the main goals of Generation IV nuclear energy systems is to minimize and manage nuclear wastes through partitioning and transmutation of transuranic elements (TRU). TRU recycling requires the availability of the reprocessing technologies that can provide separation of TRU and fission products (FP) from the spent fuel efficiently and economically. The existing industrial scale aqueous reprocessing technology using solvent extraction techniques can recover U and Pu with sufficient yields. However, high recovery yields are also required for other minor actinides if the waste management objectives are to be reached.

One of the most significant challenges in aqueous processes is the separation of trivalent actinides (An(III)) from trivalent lanthanide fission products (Ln(III)) due to their chemical similarity. Recently proposed[1-4] trivalent actinides-lanthanides separation methods are very complex therefore can significantly increase the cost of reprocessing. In this study, we investigate the basic feasibility of recycling Ln(III) fission products together with An(III) TRU without separating them as commonly assumed. TRU recycling in thermal and fast spectrum will be considered.

The objective of this study is to evaluate the effect of Ln(III) separation on major fuel cycle and core operation parameters, such as initial fissile material loadings, cycle lengths, reactivity coefficients, and TRU destruction efficiency and compare them with the similar cases where Ln(III) are separated and not recycled. The neutronic calculations will be performed with two-dimensional transport and depletion code BOXER[5] and the BGCore[6] system, currently under development at Department of Nuclear Engineering, Ben-Gurion University of the Negev.

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Factors in the Disposal of Spent Gen IV VHTR Fuel Containing Zirconium Carbide

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Zirconium carbide (ZrC) has been proposed as a component in advanced nuclear fuels for the Generation IV Very High Temperature Reactor (VHTR). Specifically, ZrC is an important fission product retention layer in tri-structural isotropic (TRISO) coated fuel particles and would replace the less refractory silicon carbide layer currently used in TRISO. However, plans for final disposition of spent TRISO fuel are undecided, with direct disposal or vitrification under consideration. Retention of fission products by the ceramic layers and minimising the volume of waste are important considerations. Also, the effects of a ZrC component in TRISO on the properties of the spent fuel must be studied to enable sound decisions on safe disposal of a fuel with novel composition and properties. This work will discuss computational and experimental methods of investigating thermal, mechanical, and thermodynamic properties affecting ZrC behaviour in VHTR fuel.

Energetic and Crystallographic Characteristics of Interstitial Dislocation Loops of Different Geometry in BCC Iron

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PACS codes/keywords: 61.72.Lk, 61.72.Ji / interstitial dislocation loops, formation energy, dipole tensor, iron, molecular statics

The formation energy, the relaxation volume, the dipole tensor and strain fields of interstitial dislocation loops in bcc iron (clusters of self interstitial atoms) have been calculated by molecular statics using interatomic interaction potential [1]. Dislocation loops of *a*/2<111><112>, *a*/2<111><110>, *a*/2<111>{110}, *a*<100><100> and *a*<100><110> types (Burgers vector and directions of dislocation segments or habit plane before relaxation) containing up to ~1100 self interstitial atoms (SIA) have been considered. Model crystallites with fixed boundary conditions containing 10^5 – $7 \cdot 10^6$ free atoms have been used for calculations.

Loops of *a*/2<111>{110} and *a*/2<111><112> types are the most energetically favorable. The formation energy difference of these loops is less than 1 eV at equal number *n* of constituent SIA. During the relaxation of the model crystallite containing *a*/2<111>{110} loop, the latter leaves the plane {110} and forms the configuration not having a single habit plane. The formation energy of *a*/2<111><110> loops is 1% greater than that of *a*/2<111>{110} and *a*/2<111><112> loops at equal *n* (100 < *n* < 1000). The formation energy of *a*<100><110> loops is 23% greater than that of *a*/2<111><112> loops. The formation energy of *a*<100><100> loops is 17% greater than that of *a*/2<111><112> loops at *n* ~100. The formation energy difference of these loops decreases to 14% with increasing of *n* to ~1000.

Energy criterion for the possibility of formation of a loop with Burgers vector **b** = *a*<100> by joining of two loops with **b** = *a*/2<111> has been proposed:

$$\Delta E = E^F_{a/2<111>}(n_1) + E^F_{a/2<111>}(n_2) - E^F_{a<100>}(n_1 + n_2) > 0 ,$$

where n_1 and n_2 are the numbers of constituent SIA of the reacting loops (clusters) with **b** = *a*/2<111>, $E^F_{a/2<111>}$ and $E^F_{a<100>}$ are the formation energies of the loops with **b** = *a*/2<111> and **b** = *a*<100>, correspondingly. Using the proposed criterion, the conclusions have been made: 1) the formation of loops with **b** = *a*<100> in iron crystal is energetically favorable at $n_1 + n_2 > 13$; 2) ΔE is maximal when the sizes of the reacting loops with **b** = *a*/2<111> are approximately equal ($n_1 \approx n_2$).

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Self-Point Defects Characteristics and Their Dependence on Stress Fields of Edge and Screw Basal Dislocations with Burgers vector 1/3$[11\bar{2}0]$ in HCP Zr

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PACS codes/keywords: 61.72.Lk, 61.72.Ji, 61.72.Yx /zirconium, self-point defects, dislocations, interactions, molecular statics, anisotropic theory of elasticity.

In hcp Zr crystal, the characteristics (formation and migration energies, relaxation volume and dipole tensor) of stable, metastable (including saddle point) configurations of self-point defects (SIA – self-intersitial atoms, vacancies) have been calculated by computer simulation methods with use of the many-body interaction potential [1]. The stress fields of the straight perfect edge and screw basal dislocations with Burgers vector 1/3$[11\bar{2}0]$ and the spatial dependence of the interaction energy between these fields and self-point defects (elastic dipoles) have been calculated using the anisotropic theory of elasticity.
The most energetically favorable SIA configuration in the attraction area of the edge dislocation is a basal crowdion (BC) oriented along the Burgers vector. Two minima of its formation energy in a given basal plane are located at the rays that make up the angles □ = 72.3° and □ = 107.7° with the slip plane (0001), and the local maximum is located at □ = 90°. The vacancy formation energy in a given basal plane is minimal at □ = 270°. The most favorable SIA configurations in the presence of the screw dislocation are BC with $[\bar{2}110]$ and $[1\bar{2}10]$ orientations. Minima of their formation energy are located at the rays □ = 270° and □ = 90°, correspondingly. The interaction energy between the screw dislocation and the stable vacancy configuration is equal to zero.
To approach to the dislocations lying in a basal plane, self-point defects have to make jumps from a basal plane to another. The most favorable mechanism for the SIA approaching to the dislocations is a combination of out-of-basal plane jump and consequent in-basal plane reorientation. As the distance to the dislocations decreases, the corresponding energy barrier increases for the SIA and decreases for the vacancy in the stated above areas of minimal formation energy of the stable SIA and vacancy configurations.

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Measurement and analysis of radioactivity induced in reactor structural materials by fission and fusion neutron spectra

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PACS codes/keywords: 24.10.-i, 25.55.-e / structural materials, neutron spectra, activation, transmutation, cooling

Low activation is one of the important parameters, which determine the choice of structural materials for fission and fusion reactors. The low-activation ferritic-martensitic steel (Fe-12Cr-2W-V-Ta-B) and vanadium alloys V-Ti-Cr are the favored concept for fusion first wall and blanket applications in the RF projects of the innovative nuclear systems. At the present time a range of compositions and an impurity level are still being investigated to better understand the sensitive of various functional and activation properties to small compositional variations and impurity level.

For the two types of the RF materials mentioned above (V-Ti-Cr alloys and 12 % Cr steels) (Russia technologies) the analysis of induced activity, hydrogen and helium-production as well as the accumulation of such elements as C, N, O, P, S, Zn and Sn as a function of irradiation time was performed. Materials “were irradiated” by fission (BN-600, BOR-60) and fusion (Russian DEMO-S Reactor Project) typical neutron spectra with neutron fluency up to 10^{21} and the cooling time up to 1000 years. The calculations of the transmutation of elements and the induced radioactivity were carried out using the FISPACT inventory code, the activation cross-section library ACDAM/ACT and the decay data library ACDAM /DEC.

It was shown that the level of impurities controls a long-term behaviour of induced activity and contact dose rate for materials. From this analysis the concentration limits of impurities were obtained. The generation of gas and solid transmutants can play a large role in changing of the properties of alloys to irradiation. Neutron-induced transmutations lead to substantial changes in elemental composition. Especially, for vanadium material the large level of solid transmutation occurs both in fission and fusion spectra. The obtained results give a complete picture about the values of induced radioactivity, dose rate, decay heat, element and gas production.

Also the results of measurements of radioactivity induced in the V, V-5Fe, V-4Ti-4Cr and V-9Ti-5Cr alloys by the BR-10 neutron spectra (Obninsk, Russia) with total neutron fluences up to 5.15×10^{25} n/m^2 were used for testing of the ACDAM activation data library. The isotope composition, activity and contact dose rate have been calculated taking into account the chemical of composition of samples, irradiation conditions and time. The comparison of experimental and calculated data was made and the contribution of the isotopes to total activity of the samples were determined. Nuclear reactions in which long-lived isotopes are produced were considered. It was shown that V, Ti, Cr nuclei do not produce long-lived isotopes except for Sc^{46} which is generated by Ti. It was established that the major isotopes, which contribute to the total activity, are produced by technological impurities: Ni, Nb, W, Re, Co, Fe, Mn, Cu, Mo.

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Development of a fuel performance code for TRISO particles in the framework of the PUMA Project

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PACS: 62.20.-x; 62.20.Mk; 25.85.-w; 28.52.Fa
Keywords: High Temperature Reactors, TRISO particles, failure probability, Pu and MA fuel kernels, thermal transmutation.

The PUMA project, a Specific Targeted Research Project of the European Union EURATOM 6th Framework Program, is mainly aimed at providing additional key elements for the utilisation and transmutation of plutonium and minor actinides in contemporary and future (high temperature) gas-cooled reactor designs [1].
The poster presents an overview of the activities of TU Delft as a participant of the PUMA project. These activities consist in improving an in-house developed fuel performance code (PASTA) for the mechanical behavior of coated fuel particles [2], including specific mechanisms for transmutation of plutonium and minor actinides in HTRs, and coupling the fuel performance code to thermal-hydraulics and neutronics codes. The objective of this integrated code system is to calculate the evolution of the fuel burn-up, fuel temperature and fast neutron fluence of the fuel pebbles during the multiple passes through the reactor core, and to use these data to calculate the particle failure fraction during the irradiation.

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Determination of the helium density and pressure in nanobubbles in implanted 9Cr-1Mo martensitic steels using electron energy-loss spectroscopy

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The aim of this work is to obtain the helium density and the pressure in small bubbles in order to identify their role in the microstructural mechanisms determining the macroscopic properties of the material. A method developed by C.A. Walsh [1] consists in measuring directly the He density from the electron energy-loss signal. Then, an appropriated equation of state (Trinkhaus' EOS [2]) can be used for calculating the pressure in bubbles from the He density. Our first observations in transmission electron microscopy show, after implantation at 550℃ with 0 .5 at% He, the occurrence of two kinds of bubbles: spherical and faceted, which we have examined separately. In the spherical bubbles, the values for the He pressure seem to be much smaller than the equilibrium pressure, and agree in trend with results of previous studies, although our results extend to smaller radii and higher pressures. In faceted bubbles the pressures tend toward the equilibrium values but are much more widely dispersed.
Further studies envisaged include the detailed examination of faceted bubbles (concerning which the literature is currently rather sparse), the selection of another implantation temperature and the development of better acquisition techniques enabling significant gains in the signal-to-noise ratios in our spectra, which are currently a limiting factor.

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TWIN ASTIR: AN IRRADIATION EXPERIMENT IN LIQUID Pb-Bi EUTECTIC ENVIRONMENT.

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The Twin Astir irradiation program, currently under irradiation in the BR2 reactor at SCK-CEN is aimed at determining the separate and possibly synergetic effects of a liquid lead bismuth eutectic (LBE) environment and neutron irradiation. It will lead to a parametrisation of the key influencing factors on the mechanical properties of the candidate structural materials for the future experimental Accelerator Driven System.

The experiment consists of six capsules containing mainly mini tensile samples and one capsule containing mini DCT's. Three of the tensile containing capsules and half of the DCT containing capsule are filled each with approximately 20 ml of low oxygen (10-6 wt%) LBE. To complete the filling of these capsules with LBE under controlled conditions a dedicated filling installation was constructed at SCK-CEN.

The other three tensile containing capsules are subjected to PWR water conditions, in order to discriminate the effect of PbBi under irradiation from the effect of the irradiation itself. To extract the effect of the PbBi corrosion itself on the material properties, one of the capsules is undergoing the thermal cycles of the BR2 reactor without being subjected to irradiation. This results in a matrix of three irradiation doses in LBE (0, 1.2 and 2.5 dpa) and two environments (PbBi and PWR water conditions).

The detailed concept of the Twin Astir project will be described as well as the materials under irradiation. We will give an overview on our experience with the experiment.

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The influence of hydrogen to fracture toughness of EUROFER steel

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Experimental results of measurements of fracture toughness of EUROFER martensitic steel in presence of hydrogen are summarized. Three-point bend method and KLST specimens were used for fracture toughness testing at room temperature and 120℃. The hydrogen effect is shown at the fracture toughness testing at room temperature both of base and weld metals. The $J_{0,2}$ integral values decrease depending on the hydrogen content in the range of 2 to 4 wppm. The hydrogen content of about 4 wppm decreases fracture toughness both of base and weld metal to the level 30 KJm^{-2} or below i.e. approx. 90 % of original values. Hydrogen containing more than 2 wppm manifests itself significantly only in base metal. At the 120℃ testing the hydrogen effect manifest itself by lower fracture toughness of base metal specimens only. The $J_{0,2}$ integral value lowers by about 30 % in the base metal at the hydrogen content approximately 1,2 – 1,6 wppm.

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Structural and electronic properties of Nb adsorption on C nanotubes

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Armchair and zig-zag carbon nanotubes (CNTs) diameter up to 1.5nm were studied by means of density functional theory (DFT). In regard to graphene C-C distances we found that the amount of structural relaxation decreases with the CNT radius, with the biggest expansion, compared to the unrelaxed system, observed for the (3,0) CNT. In agreement with previous TB calculations, the band structure calculations along the CNT axis show that all armchair (n,n) CNTs with 3<10 are metallic while some of the zig-zag (n,0) CNTs are semiconducting (n=7,8,10). In an effort to understand the growth of superconducting Nb nanowires templated by CNTs, we deposited a Nb atom on each armchair and zig-zag CNTs and we found that the energetically favoured position is over a hexagon for all cases. In addition, the presence of Nb strongly affects the first-neighbour atomic positions, especially for the smaller CNT, while the local electronic charge density of the CNT is altered showing charge transfer between the Nb adatom and the CNT. These findings could shed light on the mechanisms of the early stage growth of Nb metal on CNTs.

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NRI experience with heavy liquid metal technology

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The activities of the Nuclear Research Institute, *Division of Integrity and Technical Engineering*, can be divided into research and application contracts. Since 2001, first facility has been operated with flowing LBE in the frame ADS R&D activities at NRI Řež plc. In this time several different facilities which are working with LBE or pure Pb are operated in the frame of EURATOM 6th Framework Programme (IP EUROTRANS – domain DEMETRA, VELLA project).

The experimental activities have gone through to find the influence of interaction between the structural materials and heavy liquid metal in the field of corrosion behavior of structural materials, mechanical properties and qualification of the impurities in the system.

Corrosion studies in flowing liquid Pb-Bi are provided using corrosion convectional testing loops – COLONRI I for LBE and COLONRI II for pure Pb. The program contains the basic corrosion study of the influence of parameters such as temperature, temperature gradient, oxygen concentration, flow rate and chemical composition of materials and development and testing of oxygen sensors. Post-test examinations by microscopy (SEM, LM, TEM) and analyses of chemical compositions of structural element and surfaces are a part of the laboratory works.

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Brittle fracture of austenitic and martensitic steels induced by mercury at room temperature.

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Key words: Liquid Metal Embrittlement, plastic deformation, ferritic- martensitic and austenitic steels.

Liquid Metal Embrittlement (LME) is the transition from a ductile to a brittle rupture that requires intimate contact between the solid and the liquid metal as well as plastic deformation

Liquid Metal Embrittlement of steels by mercury (Hg) at room temperature is a technologically important subject [1, 2]. It is also of fundamental interest but little data exists on premature failure of 316L and T91 steels induced by liquid metals.

Crack growth dynamical testing at room temperature using CCT (Crack Center Tension) specimens has been carried out at different deformation rates. It has been found that 316L and T91 steels are susceptible to LME by mercury. The fractography reveal that in presence of mercury at slow deformation rates, 316L and T91 steels fail in a transgranular way, mostly by slip band decohesion. At high deformation rates, there is a ductility recovery, which is confirmed by a Crack Tip Opening Displacement (CTOD) analysis. The operating mechanism of this environmental fracture is not yet clarified.

In order to improve the understanding of the modification in fracture behavior at low deformation rate, interrupted mechanical tests in air and in mercury have been performed with the aim to nucleate a crack in Compact Tension (CT) specimens. The crack tip zone is analyzed by Electron BackScattered Diffraction (EBSD). By using this novel technique in LME study, a comparison at the mesoscopic scale between the plastic deformation behavior in air and in mercury is being investigated and preliminary results show clear indications of the plastic deformation localization induced by mercury. This analysis confirms that cracking in mercury starts at earlier stages of plastic deformation than in air. Finally, a finite element analysis of plastic deformation in presence of mercury will be presented.

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Semi-hot experimental facilities and methods employed in mechanical testing of irradiated reactor pressure vessels materials

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PACS: 62.20.Mk Fatigue, brittleness, fracture, and cracks
62.20.-x Mechanical properties of solids
01.50.Pa Laboratory experiments and apparatus
Keywords: fracture toughness, surveillance program, reconstutition, semi-hot laboratories

The main objective of this presentation is to characterise the design and construction of semi-hot cells laboratory for mechanical testing in the Nuclear Research Institute Rez. As described in this paper, the laboratory has all the necessary equipment and methods for postirradiation tensile, impact, fracture toughness and fractography measurements.

Within the Perfect subproject “Mechanics modeling”, results of mechanical properties as well as static fracture toughness results determined on the selected RPV materials in initial and irradiated conditions are summarized. Presented static fracture toughness test were carried out using shallow and deep fatigue precracked TPB specimens with dimensions 10x20 mm. For the testing, the ASTM E192105 method for reference temperature T_o determination was applied.

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Materials Selection for the High Temperature Reactor Intermediate Heat Exchanger

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PACS code: 81.00.00 Materials Science
Keywords: Alloy 617, Diffusion bonding Generation IV reactors, PCHE, FPHE

The US Generation IV Programme and other similar projects have generated considerable interest for indirect cycle gas cooled reactors. The indirect cycle gas cooled reactor produces heat at temperatures in the order of 1000℃. This heat can be used for power generation, via a Brayton or combined cycle, and hydrogen production, via a variety of high temperature processes. A key component of the indirect cycle gas cooled reactor is the intermediate heat exchanger (IHX). This paper identifies operating fluids and conditions that determine the selection criteria for the IHX. The paper concludes that appropriate material selection will be essential for this high temperature, high pressure application. Candidate materials are reviewed, with consideration given to restrictions on material availability, operating criteria, fabrication techniques and design code criteria. The review of materials would suggest that either alloy 617 or alloy 230 is the most suitable material for an IHX. In addition to the need for economic fabrication in the identified material, the selection of exchanger type will be heavily influenced by the need for a robust, high integrity, high effectiveness, compact exchanger with low pressure drop characteristics. Several generic exchanger types and their associated construction techniques are considered. It is demonstrated that the features and characteristics of a diffusion bonded exchanger type, such as the Printed Circuit Heat Exchanger (PCHE) and Formed Plate Heat Exchanger (FPHE) are ideally suited to this challenging duty. The required techniques such as diffusion bonding and passage forming for alloy 617 have been developed.

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Modelling of Radiation Damage in Austenitic Stainless Steels

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The severe and hostile operating conditions of fast breeder reactors demand the development of new materials that possess higher resistance to radiation damage. Radiation damage is a multiscale phenomenon involving processes spanning a wide range of length and time scales and necessitates use of multiscale materials modelling for understanding the behaviour of materials under irradiation. The high-energy particles collide with the lattice atoms and the resulting collision cascade produces highly non-equilibrium point defects and point defect cluster concentrations with a high degree of spatial correlation. These defects cluster and diffuse over the macroscopic time scales significantly altering the microstructure of the material, which in turn leads to some of the dimensional instabilities like void swelling and radiation creep which affects the reliability and performance of the components. Identification of radiation resistant alloys by pure experimental methods is a very tedious and time consuming exercise. Therefore modelling radiation damage would be highly useful in understanding the damage and subsequently developing the radiation resistant materials.

The paper discusses development of an ANN model to correlate chemistry, irradiation temperature, percentage of cold work and irradiation environment with void swelling. A three layer feed-forward network with back propagation learning algorithm has been employed in this study. The input parameters of the networks are the main alloying elements of austenitic stainless steel namely C, Ni, Cr, Ti, P and Si content as well as the irradiation parameters like temperature and type of environment and percentage of cold work. This gives void swelling as an output. The paper discusses optimising the configuration of the network with proper selection of hidden neurons. Further, the paper discusses the correlation coefficient of both training and test data and also analyses the sensitivity of input parameters to identify the most sensitive parameters that control radiation damage.

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Performance Assessment of a High-Level Waste Repository: Sensitivity to Environmental Factors and Radionuclide Inventories

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REPOSITORIES AS COMPONENTS

A radioactive waste repository can be one of many or one of few components in the nuclear fuel cycle. Nuclear fuel cycle models range from the inefficient but cost-effective once-through cycle to innovative approaches involving reprocessing, transmutation of waste through fast breeder reactors, and an expanding plethora of exciting options. Regardless of fuel cycle complexity, the current state of the science and technology behind the fission-based nuclear power fuel cycle dictates that fission products must be removed from spent fuel at some point.

Since fission products can remain radioactive and harmful to the surrounding environment for tens of thousands of years, it is critical to consider the complexities of both natural and engineered components of any repository. If a computer model is used to simulate the performance of the repository, it becomes important to understand what values are assumed in that model and what effect an incorrect initial guess might have on the model's output. For example, a key question in determining radiation dosage to the surrounding environment is: what are the initial radionuclide inventories? Over tens of thousands of years, other uncertain variables such as water seepage rates and corrosion rates become increasingly important.

YUCCA MOUNTAIN REPOSITORY

The Yucca Mountain Project (YMP) is the USA’s first attempt at long-term storage of High-Level Radioactive Waste (HLW). YMP seeks to incorporate HLW currently stored at over one hundred temporary sites into one repository, built in rock above the water table. Since a goal of YMP is to minimize dangers associated with long-term storage of HLW, it is important to estimate the dose rate to which current and future generations will be subjected.

Uncertainty exists as to the initial radionuclide inventories that will be stored, and it is reasonable to perform a variety of sensitivity analyses to indicate how assumed initial concentrations affect the projected dose rate to future generations. The dose rate to the maximally exposed individual is calculated based on the Simplified Total System Performance Assessment (STSPA), a model developed by Golder Associates, Inc, Booz-Allen Hamilton, Stone and Webster, and the University of Nevada Reno. The model runs on the basis of GoldSim, a user-friendly graphics-based simulation tool.

This evaluation will examine the effects of varying iodine-129 and neptunium-237 initial concentrations by two and three orders of magnitude. Such analysis indicates the consequences of incorrect estimates in the radionuclide inventories. By varying the estimated values, trends in the projected performance are observed and analyzed. The lifetime of the repository is simulated to indicate the radiation dose rate to the maximally exposed individual; it is assumed that if the maximally exposed individual would not be harmed by the annual dose, the remaining population will be at even smaller risk. The determination of what maximum levels of exposure are safe is problematic, and the results from the simulations as compared against various regulatory limits are discussed.

This sample performance assessment may provide insight as to the degree of robustness of this particular high-level waste repository. It is also interesting to compare the long-term effects of this repository against a repository which incorporates reprocessing and other waste minimization techniques.

Study of the corrosion of nickel-base alloys in molten fluorides by electrochemical methods

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Fluoride salts are contemplated for different applications such as heat carrier, electrolyte, solvent for the reprocessing of spent nuclear fuel or fuel for a molten salt reactor. The compatibility of the structural materials with the fluoride medium is a key factor for the feasibility of such processes. Metallic materials have especially to resist corrosion in fluoride salts at high temperatures. Research programs have already been performed in the 50-70's in support of the development of the molten salt reactors, in particular at ORNL (Oak Ridge National Laboratory - USA) [1, 2].

The aim of this work is to study the basis of the corrosion of nickel-base alloys in molten fluoride salts. An experimental device was designed to operate at high temperature in fluoride mixtures and to enable the use of electrochemical methods to investigate the corrosion behaviour of metallic materials.

In a first step, the charge transfers are investigated for several pure metals (Ni, Mo, W, Fe). An analytic study was carried out on the influence of the following parameters on the exchange current densities of the corrosion reactions: nature of the metal , temperature, and chemical composition of the salt. Experiments were thus performed in three different salt mixtures: LiF-NaF, LiF-CaF_2 and LiF-AlF_3 over the temperature range 900 to 1100°C.

Keywords: Molten salts, fluoride, nickel alloys, corrosion, electrochemistry,

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Positron annihilation spectroscopy study of steels pre-selected for new advanced reactor systems

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Many different materials for advanced reactor systems have been developed in past, however they have not been tested yet for new condition and therefore, a huge effort must be carried out for their characterization and validation in the R&D phase. Moreover, the issue concerning the structural integrity of materials is going to have a more and more dominant role due to the degradation mechanisms, which must be understood in order to estimate the component lifetime. This work presents some interesting results on few candidate materials selected for advanced reactors systems. The study is based on application of positron annihilation spectroscopy to investigate materials as EUROFER'97, P91 and T91.

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Structural materials for advanced nuclear systems studied by non destructive techniques

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Different Fe-Cr alloys with the steels T91, P91 and Eurofer97 as reference materials were studied in details using various approaches. Positron annihilation lifetime spectroscopy PALS in combination with Transmission electron microscopy (TEM), Mössbauer spectroscopy (MS) and X-Ray Diffraction (XRD) were applied. The experimental based on implantation of H and He ions were performed for study of radiation damage effects. Implantations were performed on cascade accelerator at different doses according to previous SRIM code simulations and DPA calculations. This works present first XRD and PALS measurements in as received state and after He implantations. Results shows observable changes in coherent domain size between different Cr content alloys. This phenomenon was observed in increasing dose of implanted He ions as well.

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Phase Field Modeling of the Effect of Irradiation Damage on Thermal Conductivity at the Microstructural Scale

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A critical materials issue for all nuclear reactor systems, including Generation IV reactors, is the degradation of thermal conductivity due to irradiation damage. For instance, the ever-decreasing thermal conductivity of the nuclear fuel due to increasing porosity can eventually lead to overheating of the central part of the pellets during use. In this work, we perform mesoscale computer simulations in order to better understand how porosity as well as microstructural evolution (i.e., grain growth) effect the thermal conductivity of nuclear fuel as well as structural materials.

Phase field modeling is used to simulate grain growth in polycrystalline systems containing finely dispersed voids of varying size and volume fraction that induce a pinning effect on grain boundary migration [1]. At any specific time step, the overall temperature distribution of the microstructure throughout time is determined by solving a variable-conductivity Poisson equation, in which grain boundary and void regions are assigned reduced and zero conductivity, respectively. The finite difference method using a rectangular grid of several million points is used to discretize the governing equations and the solution is obtained using massively parallel computing.

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Microstructure research of nuclear materials at IAP NASU

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PACS numbers: 02.50-r, 05.20.Gr, 05.40.-a
Key words: complexity, hierarchical ensemble, hierarchical tree.

Institute of applied physics deals with both experimental and theoretical researches of nuclear materials. A new scanning nuclear microprobe based on a single-ended 2 MV Van de Graaff accelerator has recently been designed and constructed at IAP NASU [1].

Theoretical researches of a microstructure of nuclear materials are devoted to the description of defect structures. In addition to well-known characteristics type of hardness and elasticity limit the theoretical scheme is developed, which allows one to determine complexity of hierarchically constrained defect structures. These investigations are based on original theory of hierarchical statistical ensembles [2]. Within the framework of this theory, statistical distribution over levels of hierarchical ensemble of different defects in crystals is found. As a result, the measure of disorder of statistical ensemble of defects is defined. The states of this ensemble are distributed over hierarchical tree nodes for different values of branch index. It is shown that hierarchical structure increases the statistical ensemble complexity up to boundary value with both increase of hierarchy levels number and redistribution of non-stationary states in the course of the time. Increasing of hierarchical tree branching leads to monotonous grows from zero to infinity. With variation of statistical ensemble variance the appropriate behavior, being typical for simple systems, observes when the branch index is larger then gold mean. On the other hand, the complexity decreases with the ensemble variance growth when the branch index less then gold mean.

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Radiation embrittlement of reactor pressure vessel steels with a high nickel content

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Keywords: RPV steel, surveillance tests, radiation embrittlement, nickel, fracture toughness, Master curve
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The analysis of the Ukrainian NPP surveillance test results for the VVER-1000 reactor pressure vessel has been performed. A nickel effect on RPV material embrittlement was considered taking into account a manganese content. It is shown the radiation embrittlement rate for welds with a high nickel (> 1,5 % wt) and high manganese (> 0,8 % wt) content exceeds a normative value. Fracture toughness data for the RPV steels have been re-evaluated using the Master curve methodology. The conclusion was made the critical brittleness temperature shift due to irradiation, ΔT_F, may underestimate the fracture toughness curve shift. Furthermore, it has been demonstrated the PNAE G-7-002-86 normative approach characterizes highly conservatively the fracture toughness of some unirradiated RPV materials.

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Simulation of Corrosion Properties of MSR related Ni-Mo alloys in Molten Fluoride Salts using Electron Beam Irradiation

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Keywords: Hastelloy alloys, Neutron irradiation, Electron-Gamma irradiation, Molten salt reactor, Corrosion

In recent experiment [1] using the KIPT Electron Irradiation Test Facility (EITF) strong impact of 10 MeV (e^-,□) irradiation on the corrosion rates of the Hastelloy N type Ni-Mo alloys in the NaF-ZrF_4 fluorides melt at 650 ℃ has been revealed. To eva luate the applicability of these data for prediction of alloy corrosion at irradiation environments of G-IV MSR, we perform the Monte Carlo calculations of energy deposition and primary radiation damage rates at alloy–melt interfaces using both a model of the EITF EB experiment and a set of parametric models of MSR cores with different spectra of neutron and gamma fluxes. Impact of alloy irradiation by the fuel fission fragments in MSR is also taken into account.

The results of the EITF/MSR modeling performed by means of the same CERN GEANT4 based novel Monte Carlo code, *RaT*, show that :

- effect of some alloy constituents (Mo, Mn, Al) can be essential with respect to nuclear heating of alloys under MSR long-term irradiation when the decay heat due to alloy neutron activation has to be taken into account;
- gamma heating is a predominant factor of energy deposition in MSR irradiated alloys except for the cases of alloy interfaces with fissile MS fuel when heavy fission fragments make major contributions both to heating and radiation damage of surface layers;
- comparable energy deposition rates are achieved at 10 MeV 520 □A EITF EB irradiation and for MSRs with core neutron flux of 10^{14}–10^{15} $cm^{-2}\cdot s^{-1}$;
- the alloy dpa rate is ~10^3 times higher in MSRs than in EITF; to some extension this difference can be accounted using proposed scaling of the fluxes controlling the corrosion.

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Amorphization Kinetics under Electron Irradiation

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Keywords: amorphization; electron irradiation; interphase boundary.

Electron irradiation affects the kinetics of phase transformations not only because of the diffusion increase due to Frenkel's pairs production, but also due to activation processes at the interphase boundaries. In paper [1] a new model for the kinetics of phase transformations under electron irradiation was developed. We apply it to consider the electron-irradiation-induced amorphization as a particular case.

We assume that nucleation of a new phase occurs due to accumulation of radiation damage in defective regions, including e.g. point defects complexes, a dislocation core sector, a boundary, a triple joint or other structure defects which substantially increase the local free energy. The growth (dissolution) rate of an amorphous precipitate contains contributions both from thermodynamic driving force and relaxation of irradiation-induced nonequilibrium atomic configurations at the crystal-amorphous boundary. These contributions are denoted u_{th} and u_{irr} respectively:

$$u \equiv dR/dt = u_{irr} + u_{th}\,, \qquad (1)$$

where R is the radius of an amorphous precipitate. We argue that contributions u_{irr} and u_{th} have different signs. The thermodynamic driving force "pushes" the boundary atoms to the phase with the minimal free energy (the crystalline one). Irradiation, on the contrary, "pushes" the atoms to the amorphous phase, if the probability of relaxation of the nonequilibrium boundary atomic states into the amorphous phase is higher than into the crystalline one. Therefore, the next criterion for the irradiation-induced amorphization is obtained:

$$u_{irr} > -u_{th}\,. \qquad (2)$$

Using criterion (2), the critical electron flux, needed for amorphization at a certain temperature, and the irradiation dose required for amorphization are derived.

The formulae derived are applied to fit the experimental results on the electron-irradiation-induced amorphization of Zr_3Fe [2].

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Grain Growth in Nanocrystalline Metals under In Situ Ion-Beam Irradiation

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Keywords: Ion irradiation, nanocrystalline, grain growth, thermal spike
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Ion-irradiation-induced grain-growth in nanocrystalline metals was studied systematically using i*n situ* experiments, and a theoretical model was developed to explain the results. Free-standing Zr, Pt, Cu and Au, Cu-Fe, and Zr-Fe nanocrystalline thin-films prepared by sputter-deposition were irradiated in-situ at the Intermediate Voltage Electron Microscope (IVEM) at Argonne National Laboratory with Ar and Kr ions to fluences in excess of 10^{16} ion/cm^2 at temperatures ranging from 20 to 773 K. The grain growth was followed *in situ* by systematically recording bright-field images and diffraction patterns at successive ion-irradiation doses. Grain growth was observed as a result of irradiation in all samples at all irradiation temperatures with three regimes: (i): a low temperature regime (below about 0.15 to 0.22 T_m) where grain-growth does not depend on the irradiation temperature, (ii) a thermally assisted regime where both the grain-growth rate and the final grain size increases with increasing irradiation temperature, and (iii) a thermal regime where thermal effects dominate ion beam effects.

In the low temperature regime ion-irradiation induced grain-growth data could be best fitted with curves of the type: $\mathbf{D^n - D_0^n = K\Phi}$ with n~3. For this temperature-independent regime a model of grain-growth under ion irradiation was developed, based on direct impact of irradiation-induced thermal-spikes on grain-boundaries. In the proposed model, grain-boundary migration occurs by atomic jumps within the thermal-spike biased by the local grain-boundary curvature driving-force. The model incorporates cascade structure features such as subcascade formation, and the probability of subcascades occurring at grain-boundaries. This results in a power law expression relating the average grain-size with the ion dose, where the exponent of 3 is recovered, in agreement with the experimental data. The model also explains the differences of grain-growth rate between the different alloys.

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Characterization and in-situ Fe ion irradiation of four MA-ODS steels of interest for structural applications in GEN-IV nuclear reactors

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Oxide dispersion strengthened (ODS) ferritic steels produced by mechanical alloying techniques are considered as possible structural materials for the next generation (GEN-IV) of nuclear reactors. They are expected to achieve high creep strength thanks to the incorporation of a very high density of fine-scale oxide particles in the matrix, and be resistant to radiation swelling. Since these alloys derive most of their properties from the presence of this fine dispersion of particles, to predict their performance, a detailed characterization of the nano-sized particles must be performed and their stability under irradiation must be assessed. We present here the characterization study of the as-fabricated microstructure and dispersion particles, as well as the microstructure evolution and the behavior of these particles under *in-situ* Fe ion irradiation in an electron microscope.

For this study, various alloys were selected among the many MA-ODS steels available. The materials included two heats of MA-957 (from two different manufacturers), MA956, the French alloy DY, and the Japanese alloy M16 ODS steel (JNC). The materials were characterized in the as-received state using synchrotron radiation diffraction in reflection geometry, (the synchrotron radiation being capable of detecting small volume fractions of precipitates). None of the alloys exhibited diffraction peaks associated with the oxide dispersoids (yttria or titania) initially introduced, suggesting that they have been dissolved or changed their structure during processing. Depending on the alloys, the XRD analysis also showed the formation of intermetallic precipitates (such as the χ phase in the DY alloy) and mixed-metal carbides (of the form $M_{23}(W,Mo)_2C_{12}$ in the JNC alloy). Also, TEM samples were processed by electropolishing to characterize the overall grain size/morphology of the alloys as well as the precipitate morphology and size distribution. For instance, these examinations showed two populations of oxides size-wise (very fine particles (few nms) vs. larger ones (few hundreds of nms) in every alloy, differences in the grain morphology etc.

As a first step to understanding in-reactor behavior, irradiation with ions is an effective means to investigate the stability of the nano-particles under irradiation. Therefore, in-situ Fe ion irradiations were conducted at the Intermediate Voltage Electron Microscope (IVEM) at Argonne National Laboratory using 300 keV Fe ions at both room temperature and 500ºC to more than 10 dpas At room temperature, some precipitates seemed to amorphize under irradiation while at 500ºC they appeared to be more stable, indicating that temperature is an influential parameter in determining the stability of these particles. Future work includes more irradiations of these materials at higher temperatures relevant to GEN-IV reactor operating conditions (500ºC-800ºC).

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