The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
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IAEA
International Atomic Energy Agency

2137-5

Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for Characterization and Basic Understanding of Radiation Damage Mechanisms in Materials

12 - 23 April 2010

Multi-Scale Modelling for Characterization and Basic Understanding of RD Mechanisms in Materials

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Joint ICTP/IAEA Advanced Workshop on

ICTP Trieste, 12-22 April 2010

Multi-Scale Modelling for Characterization and Basic Understanding of RD Mechanisms in Materials

Andrej Zeman

NAPC / Physics section

IAEA

International Atomic Energy Agency

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International Atomic Energy Agency (IAEA)

Atoms for Peace (1953) addressed by D.Eisenhower, to the 470th Plenary Meeting of the UN GA

- **Founded 1957**
- HQ in Vienna
- **150 Member States**
- 6 Divisions
- 2200 Staff
- About 300 MEuro Budget
- www.iaea.org

Pillars of the IAEA

- Promoting Science & Technology

  the world's focal point to mobilize peaceful applications of nuclear science and technology for critical needs in developing countries

- Promoting Safeguards & Verification:

  the world's nuclear inspectorate

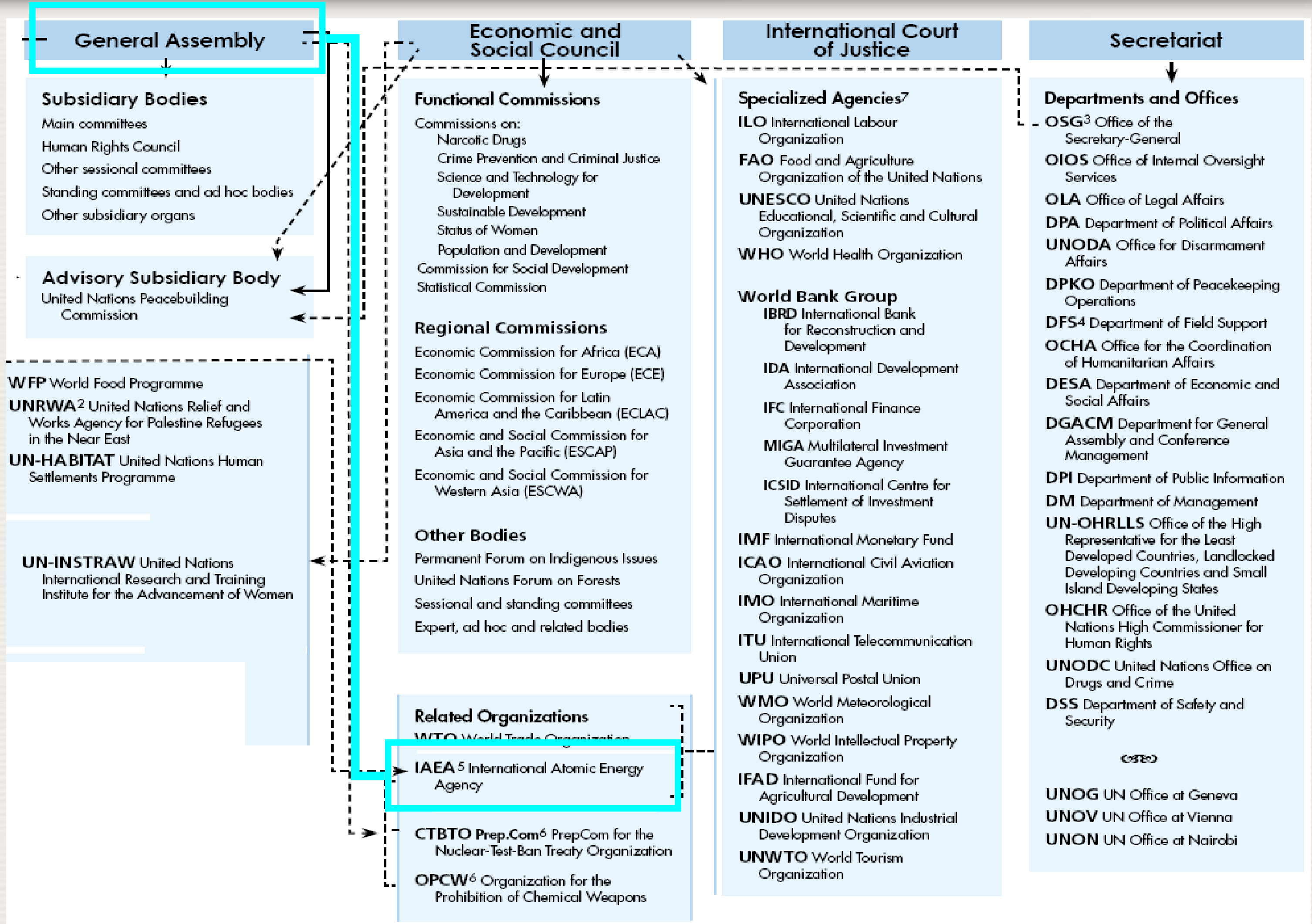
- Promoting Safety and Security

  helps countries to upgrade nuclear safety and security

IAEA's 50 Years of Atoms for Peace (2007)

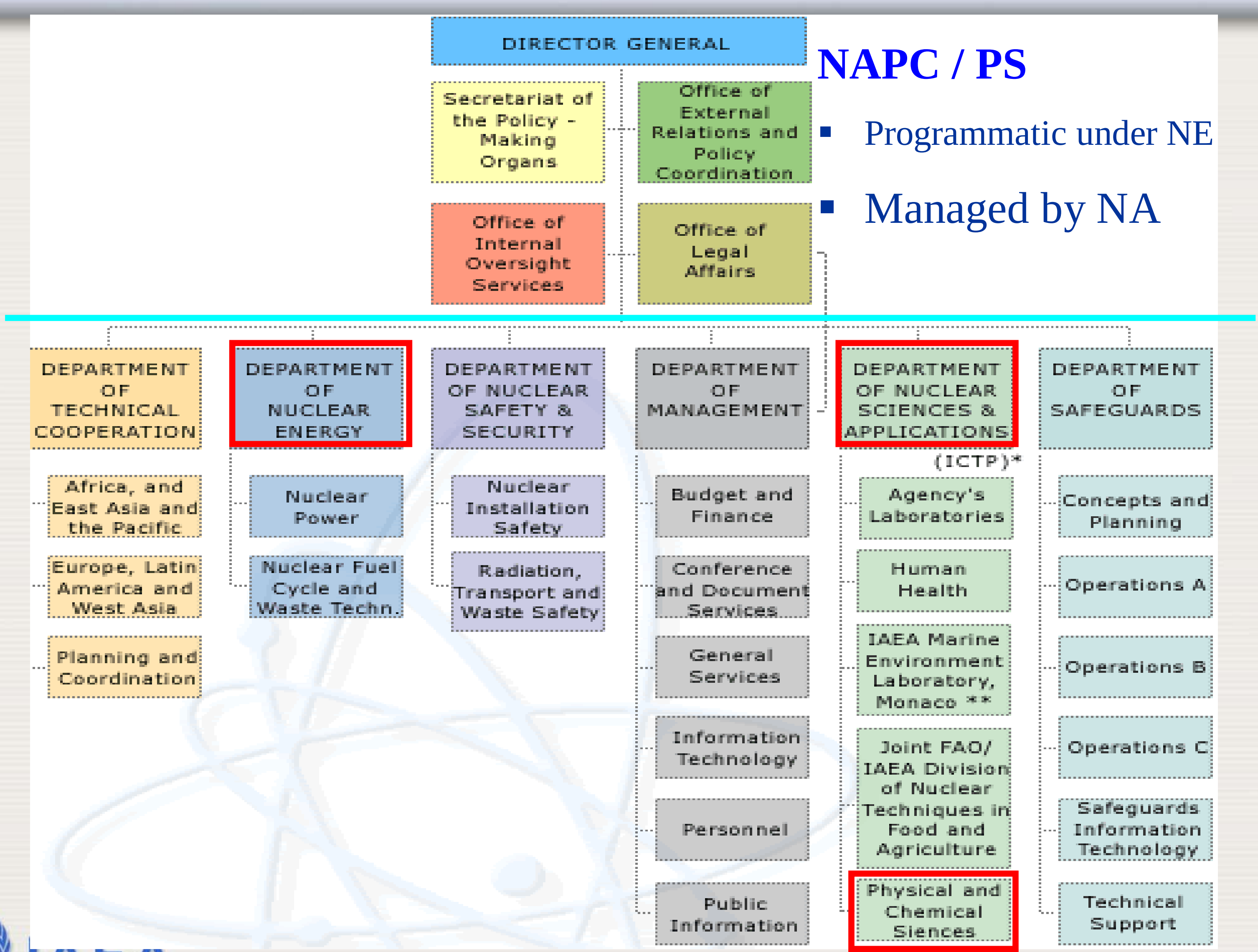
IAEA

IAEA in UN system



IAEA

IAEA organizational chart



NAPC / PS

- Programmatic under NE
- Managed by NA

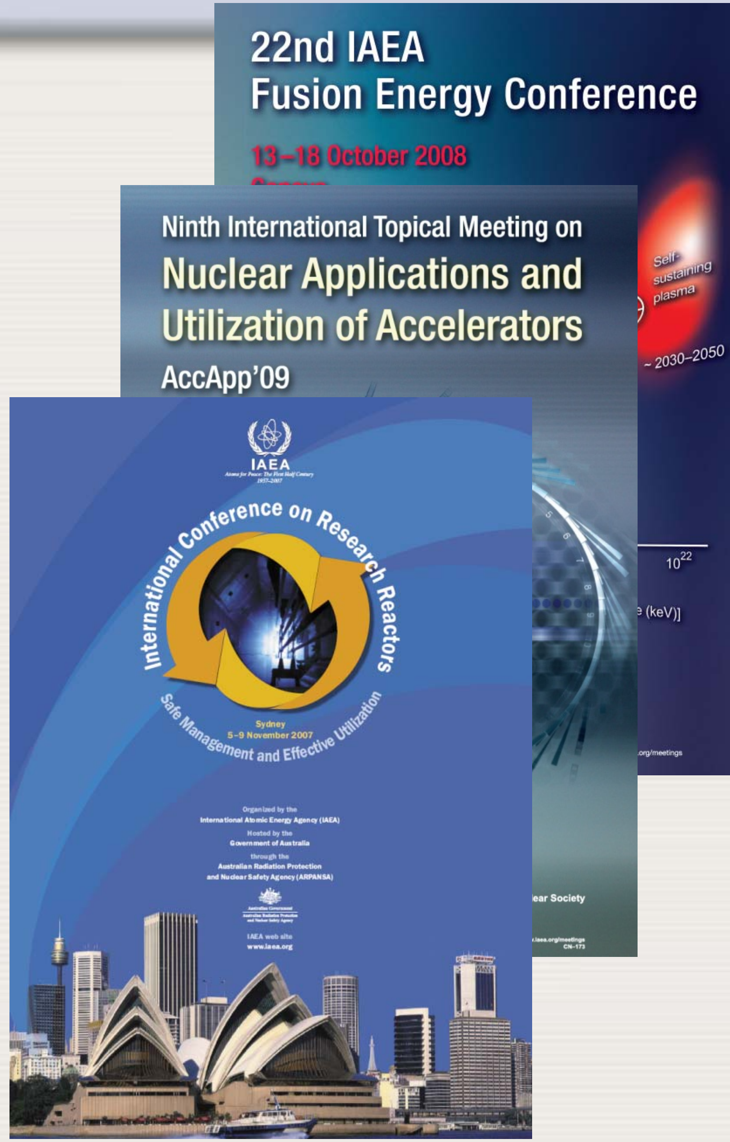
IAEA

Profile of the Physics Section

The PS supports the IAEA Member States regarding utilization of:

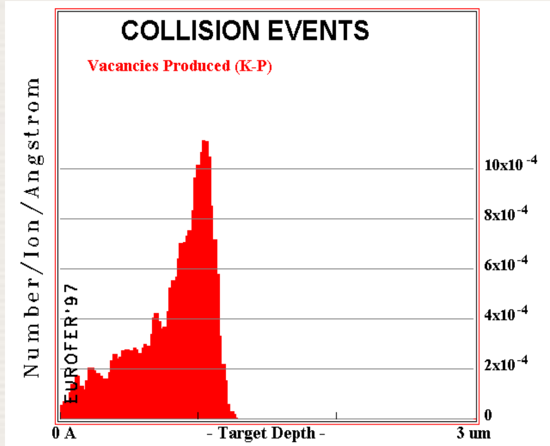
- ❑ Accelerators
- ❑ Research reactors
- ❑ Cross-cutting material research
- ❑ Controlled fusion
- ❑ Nuclear instrumentation

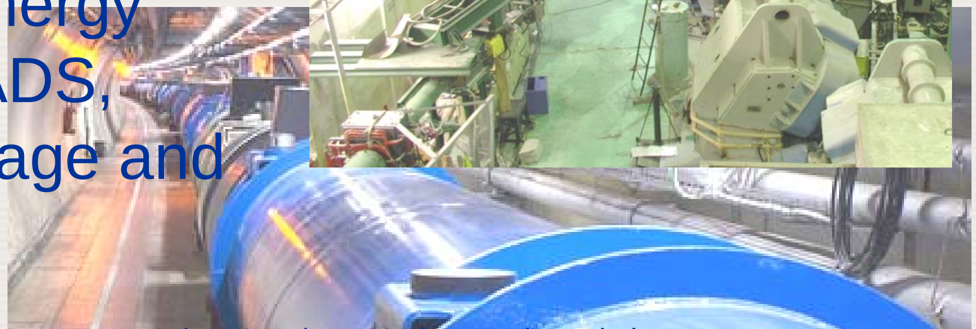
PS implements P&B activities based on MS demand: Int. conferences, TM, Experts' meetings, Coordinated research, Networks, DBs, TC, etc.



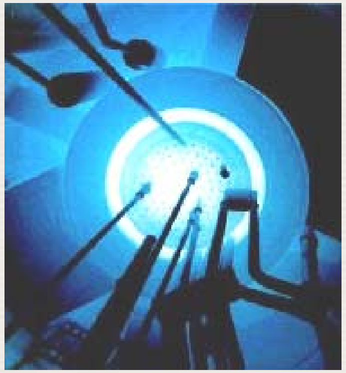
Application of accelerators:

- Accelerators and its application in multidisciplinary research and industry.
- Small and medium size facilities; particle and X-ray machines (CC scheme)
- Various probing methods (IBA, PIXE, PIGE, SAXS, etc.)
- Focus on development of advanced materials and simulation of various processes, primarily for energy systems (fission, fusion, ADS, hydrogen production, storage and conversion)





Applications of RRs:



- Irradiation programs (radio-isotopes, R&D structural materials, nuclear and non-nuclear energy applications)
- HR development (Training activities, know-how dissemination, professionals & students)
- Support of basic & applied research (neutron physics, material science, industrial applications)
- Other areas (biology, medicine, semiconductors, hydrogen economy: production, storage and conversion).

PS activities – programmatic view

Activities linked with the rationale of IAEA's program:

- 1.4.2.1 (D2) Enhancement of utilization and applications of RRs, promote the continued development of scientific research and technological development using research reactors.
- 1.4.3.1 (D3) Accelerator techniques for modification and analysis of materials for nuclear, analytical and computational investigative tools, on the engineering front - new material performance testing technologies,
- 1.4.4.1 (D4) Supporting plasma physics and fusion research, support of advanced devices operating plasmas that are used for materials research and industrial applications.

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Role and mandate of IAEA

53rd IAEA General Conference, Vienna, 14-18 Sep 2009

- Agency should encourage and assist research and development and practical application of atomic energy for peaceful uses and to foster the exchange of scientific and technical information
- Support bilateral and international initiatives and their joint R&D on innovative approaches to nuclear power
- Secretariat has to promote the exchange of relevant technical information among interested MS and foster HR trainings
- IAEA should identify and explore innovative institutional and infrastructural solutions supporting the future deployment of innovative nuclear energy systems
- Coordination and strengthening of research activities among MS (e.g. CRP, WGs, Expert meetings, etc.)

NPP structural materials - RDM

Physical protection functionality

- System of barriers (FP): Fuel matrix - Cladding – Reactor (PL) – Containment
- R(P)V – key component (non-replaceable), LWR (Gen II+ from 1980's) designed 40y, some operators plan to extend up to 60 (80y).
- Structural materials - have to assure all (designed) parameters of component and they are directly linked with its functionality!
- Reactor core components – degradation due to ageing and other external factors (radiation, temperature, chemistry, etc.), it's linked with component reliability
- RD mechanisms: embrittlement, thermal creep, swelling, cracking, etc. to be carefully considered in design phase (engineering approach)
- Need to understand material behaviour at least in range of designed limits!

Zeman et al., Int. School of Physics (ITEP), Moscow, 12-18 February 2007

On-going issues & int. cooperation

- Activities at the level of basic research should be more open, there is no general coordination on material development (budget issues, fusion (EFDA) different approach).
- New multidisciplinary approaches, effective application of lessons-learned, role of the theoretical modelling should not be over-estimated.
- Stimulation of basic R&D and int. coordination of individual on-going initiatives (intellectual property rights).
- Support of basic R&D to be addressed – invitations via broader research community (Academia and Universities).
- Closer interaction with other Int. organizations is needed (GIF, SNETP, EERA, BA, ITER, IEA-FA…).
- IAEA recognised as a focal point, Agency supports all 150 MS.

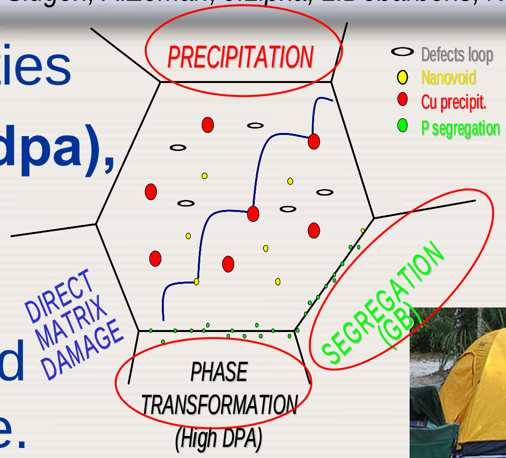
Main issues – radiation damage

V. Slugen, A.Zeman, J.Lipka, L.Debarberis, NDT&E Int. 37 (2004) 651-661

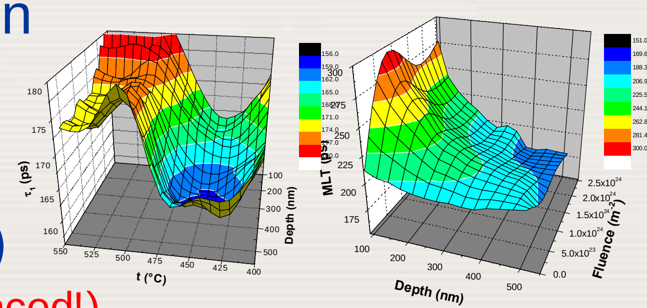
- Direct impact on mechanical properties
- Effects like: Direct Matrix Damage **(dpa),** Precipitation, Segregation, Phase transformation, etc.
- Alloying elements (Ni, Mn, Cr, V) and impurities (Cu, P) play important role.
- Thermal (Q) and mechanical treatment (CR) can accelerate or reduce such processes (e.g. impact on distribution and size of grains).
- Effect of Flux (dose rate), energy spectra (En > 0.5 MeV) and temperature.
- Higher doses (> 10 dpa) – Transmutation

LWR: RPV ~ 0.1 dpa, RVI (up 10 dpa)

(1 dpa = every single atom in lattice has been displaced!)

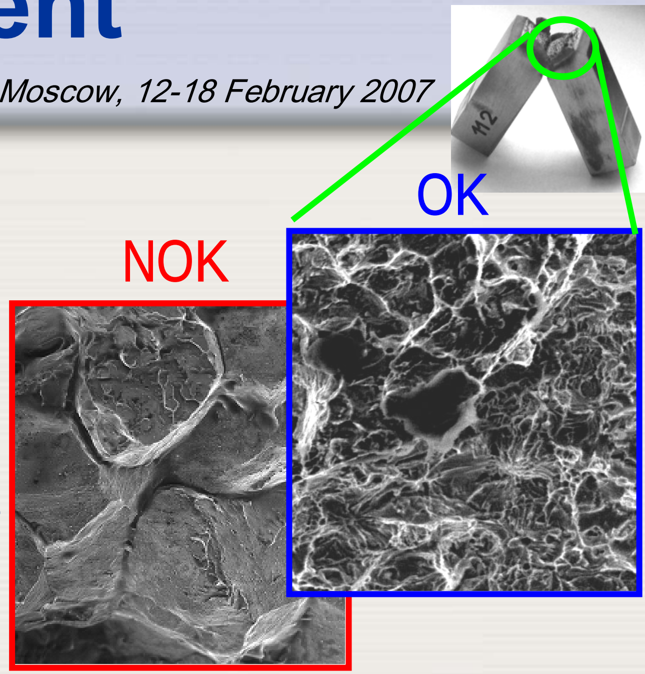


Luckily, lattice behaves differently, recovery mechanisms, however only under certain conditions!



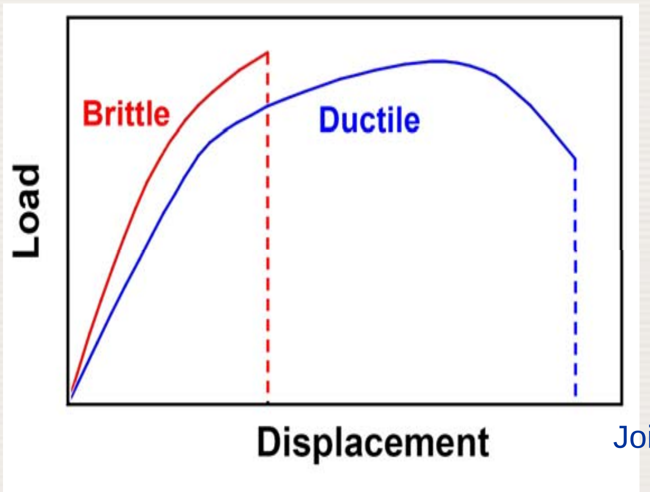
Main issues – embrittlement

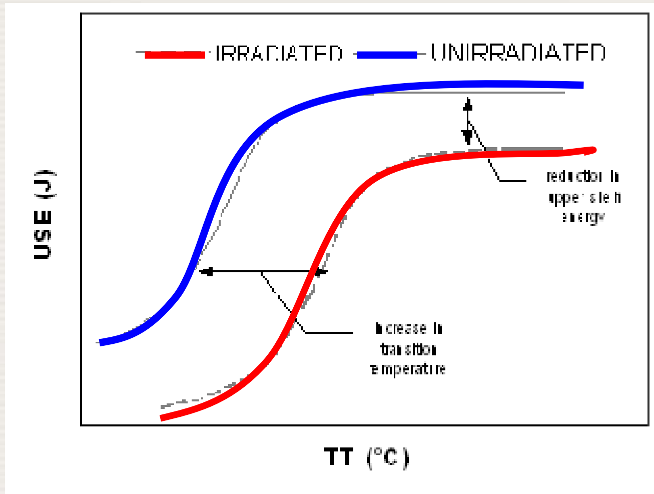
Zeman et al., Int. School of Physics (ITEP), Moscow, 12-18 February 2007



Serious problem for RPV (non-replaceable)

- Normal (ductile) fracture occurs by direct breaking of atomic bonds along the crystallographic planes
- Brittle fracture spreads through the grains and grain boundaries because grains are oriented in different directions, crack changes direction at the grain boundary
- DBTT limits RPV operation!



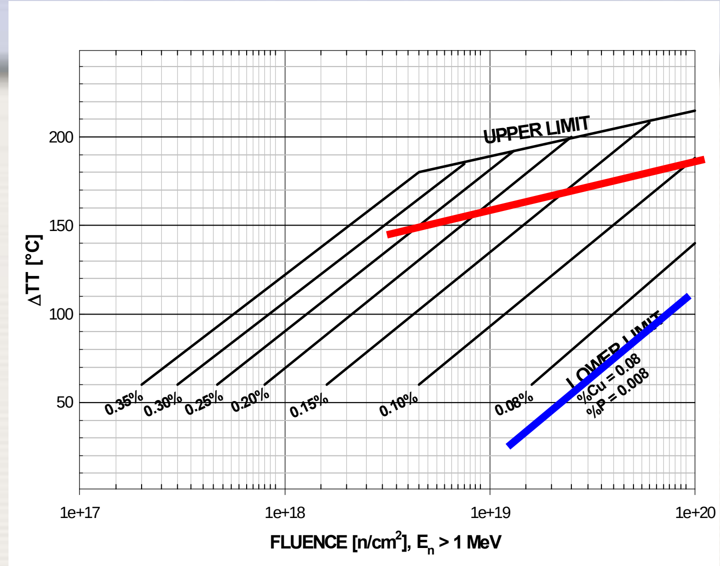


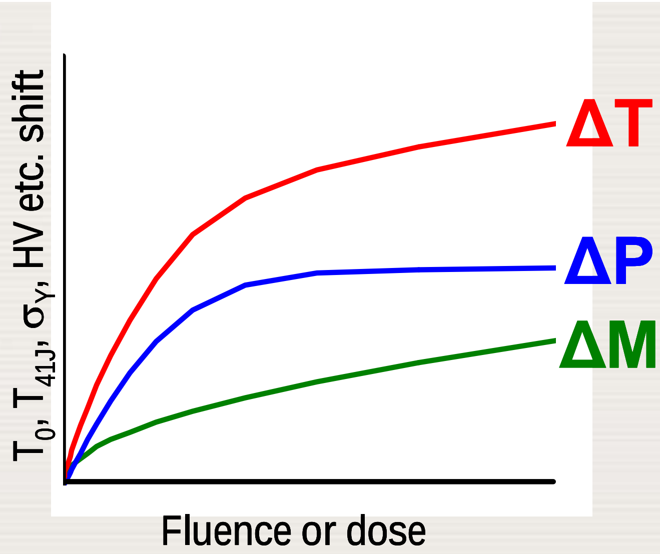
Main issues – prediction models

- Mechanical (macroscopic) properties - consequence of micro-structural changes
- Prediction models - designed for EOL
- Safety margins vs. lifetime extensions
- Study of microstructural mechanisms - more precise models
- Benefits for future innovative reactors (fission and fusion)

ΔT = ΔM + ΔP

Total = Matrix + Precipitation





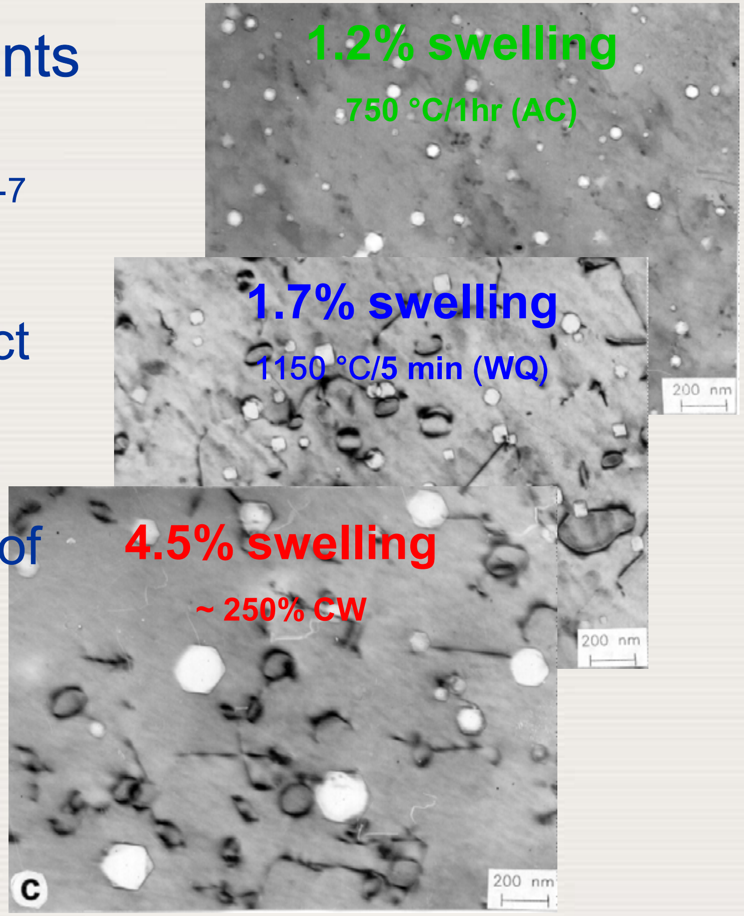
Zeman et al., Int. School of Physics (ITEP), Moscow, 12-18 February 2007

Main issues – swelling

Garner, IAEA Satellite meeting on Cross-cutting issues of structural materials for fusion and fission applications, ICFRM-13, Sapporo (Japan), 10-11 September 2009

Issue for fuel cladding and core components

- Void swelling in Fe irradiated in the BR-10 fast reactor at 400°C to 25.8 dpa at 4 x 10^{-7} dpa/sec
- Variations in neutron flux-spectra can affect property changes via transmutation rates and dpa rates.
- While recognized as important the impact of these effects has often been strongly underestimated.
- Traditionally, predictive swelling equations for steels have ignored these effects

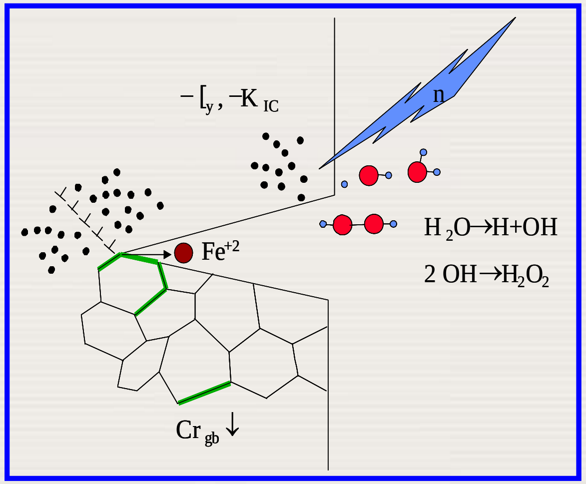


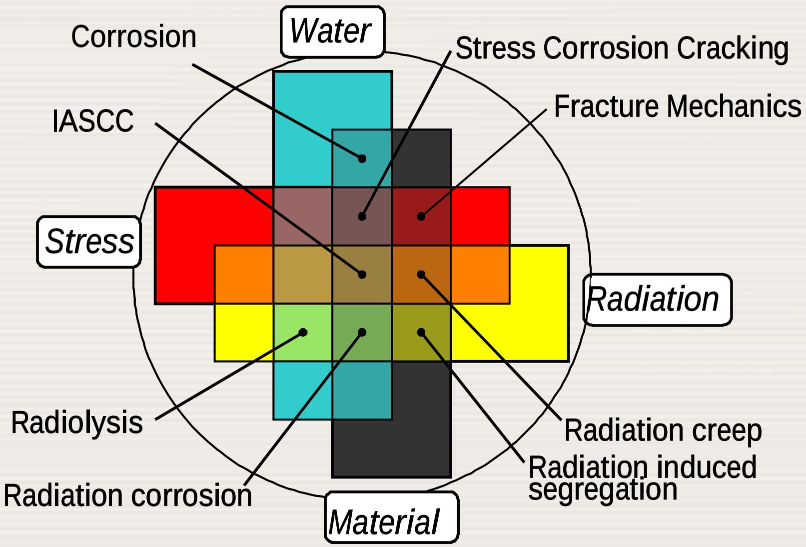
Long-accepted formula (AISI304): % swelling = A(T) $(dpa)^2$
Now-accepted version: % swelling = A $(dpa\ rate)^{-0.731}$ $(dpa)^2$

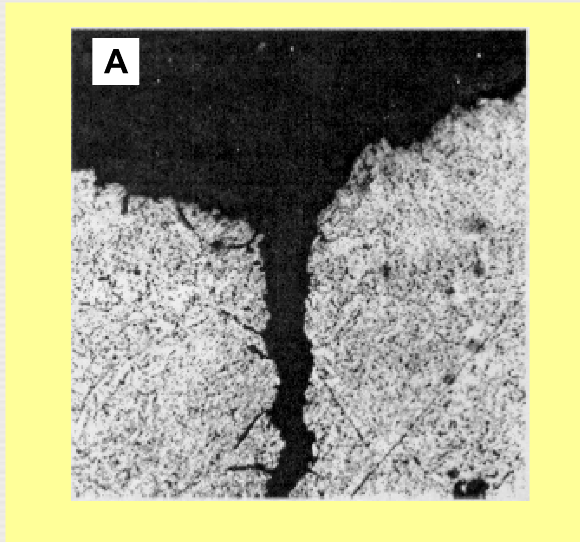
Main issues – (micro)chemistry

Debarberis et al., IAEA-ICTP Advance Workshop on Development of Radiation resistan materials, ICTP Tieste, 20-24 April 2009

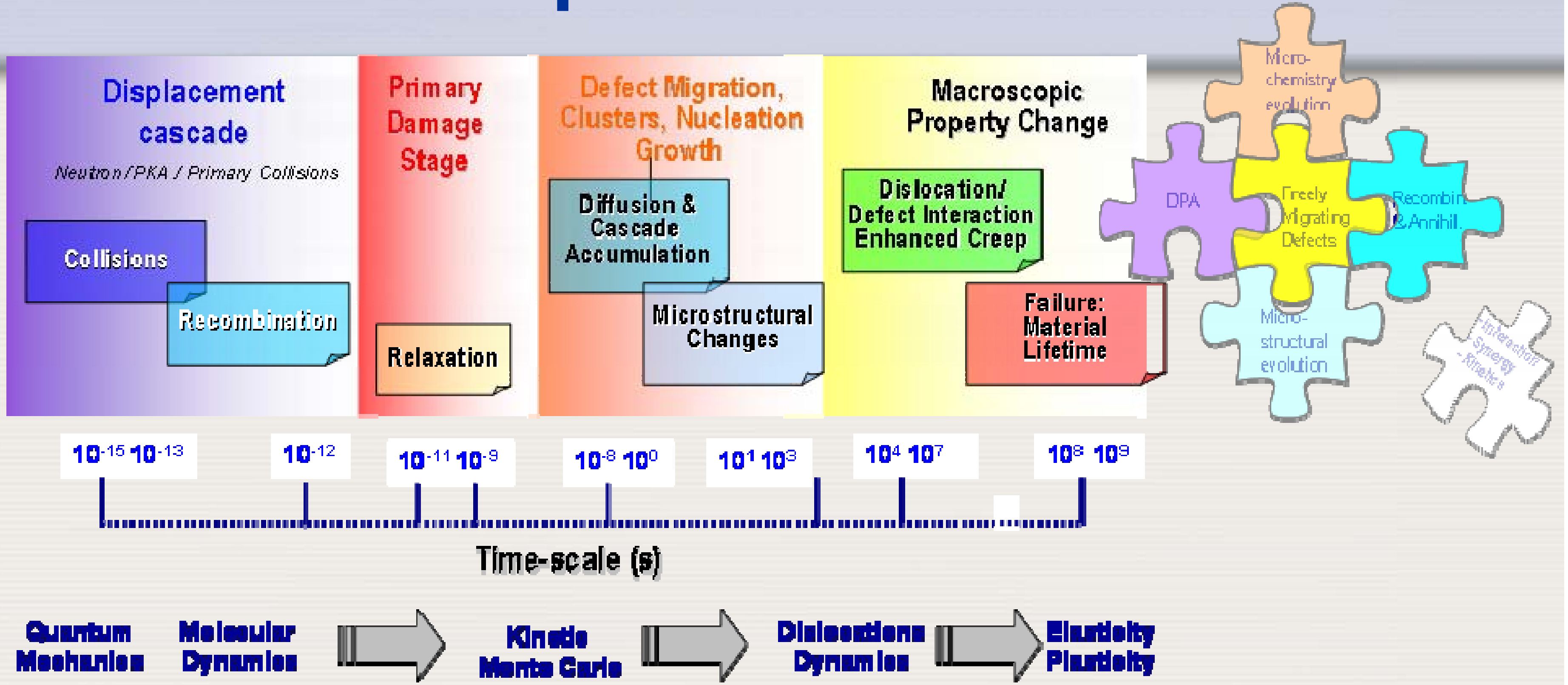
- Irradiation assisted stress corrosion cracking (IASCC)
- RVI issues (dose > 10 dpa)
- LWR Serious problem (RVI), high coolant flow rate (thermo-hydraulic stress)
- Chemistry extremely important (O, H)



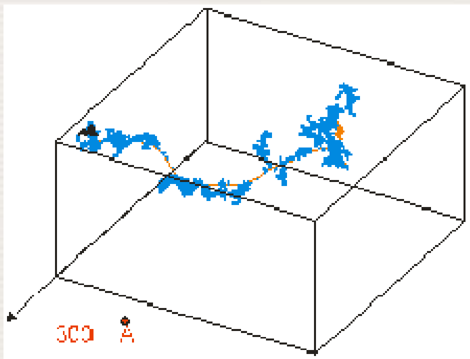


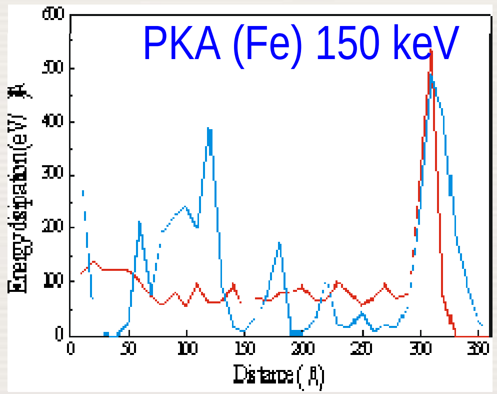


Main issues – prediction models



- Multiscale approach
- Ab-initio calculations of PKA & SKA
- Vacancy clusters formation
- Energy transfer to the lattice





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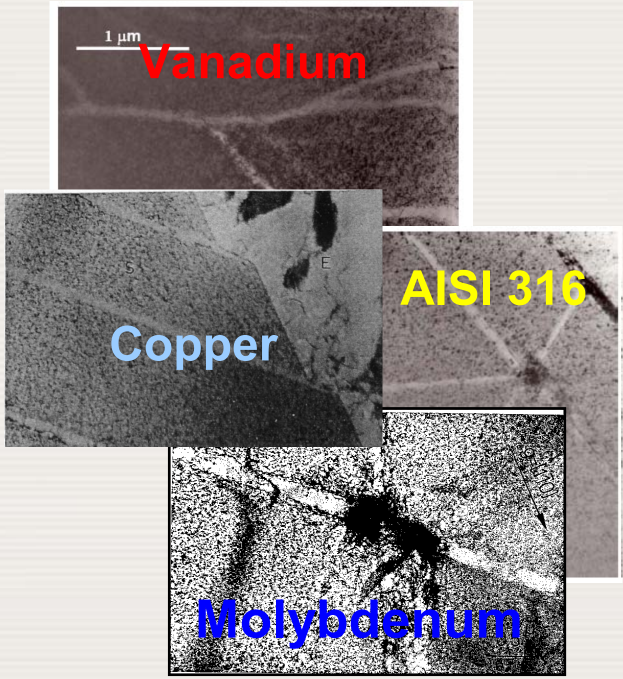
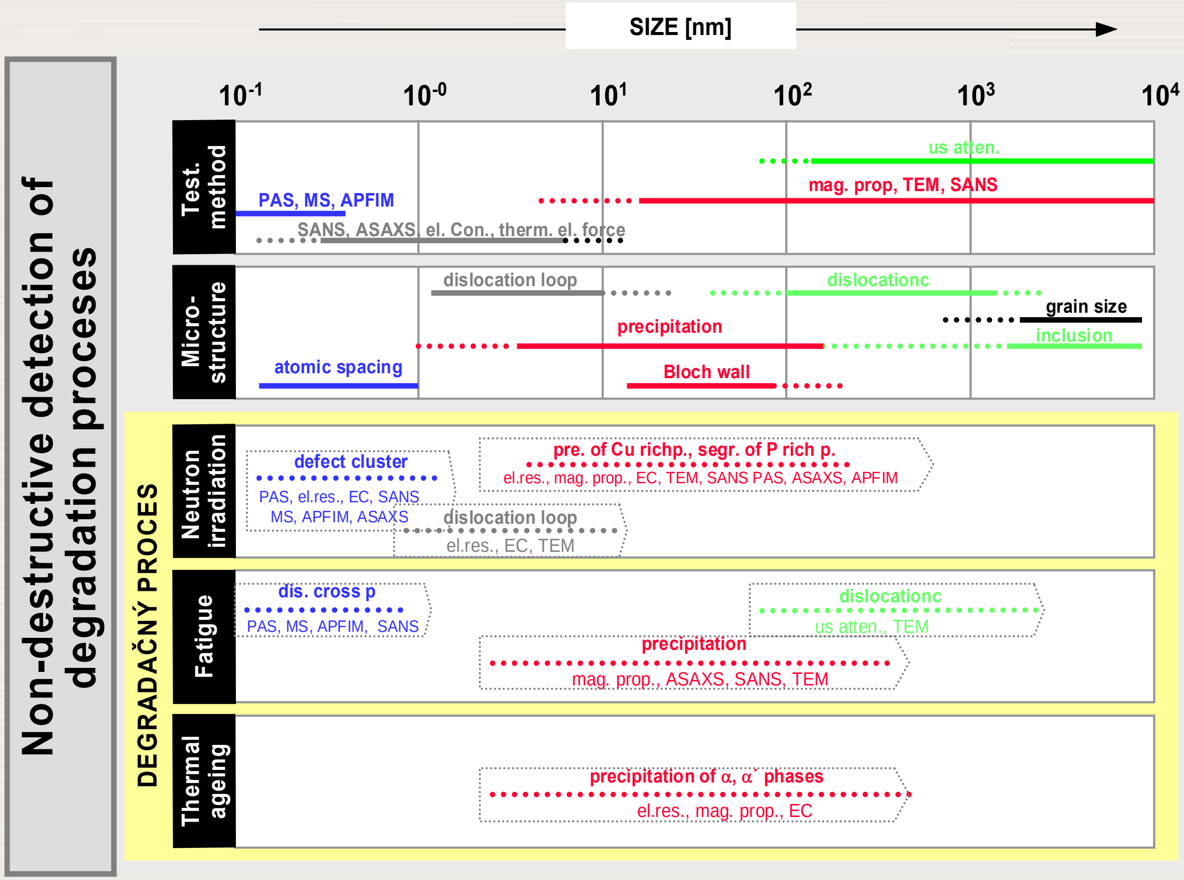
Main issues – Experimental validation

Microstructural evaluation: Localized deformation (e.g. dislocation channeling, phase transformation, etc.) occurs in irradiated metals (alloys)

Zinkle, IAEA-ICTP Advance Workshop on Development of Radiation resistant materials, ICTP Trieste, 20-24 April 2009





Zeman et al., Int. School of Physics (ITEP), Moscow, 12-18 February 2007

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Recent R&D activities

- Last decade, R&D activities driven by fusion community, ITER and non-ITER countries contributed to studies of RDM.
- Continuous development of semi-mechanistical and multi-scale models, especially in terms of radiation degradation mechanisms (RPV, RVI and fuel).
- Multi-disciplinary approach, effective application of lessons-learned (advanced metallurgy, aerospace industry, nano-science…).
- Prediction models will be crucial in future material development, however at the moment, role of the theoretical modelling should not be over-estimated, experimental studies are needed.


Coordinated Research Activities Website - Windows Internet Explorer
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Coordinated Research Project (on-going)

IAEA CRP on Accelerator Simulation and Theoretical Modelling of Radiation Effects (jointly NA-NE)

Deals with several issues related to the proton and ion beam irradiation in order to achieve very high radiation damage, project aims to facilitate following issues:

(1) Better understanding of radiation effects and mechanisms of material damage and basic physics of accelerator irradiation under specific conditions,

(2) Improvement of knowledge and data for the present and new generation of structural materials,

(3) Contribution to developmental of theoretical models for radiation degradation mechanism and

(4) Fostering of advanced and innovative technologies by support of round robin testing, collaboration and networking.

Coordinated Research Project (on-going)

IAEA CRP on Accelerator Simulation and Theoretical Modelling of Radiation Effects (jointly NA-NE) - FACTS

Extensive theoretical and experimental studies are being carried out among participating laboratories form Belgium, China, European Commission, France, India, Japan, Korea, Kazakhstan ,Poland, Russia, Spain, Slovak Republic, Ukraine and USA (18 full members).

- Project launched 01/2009
- First reporting point is RCM to be hosted by CEA (Paris) 05/2010
- Members will present recent achievements on experimental testing of various ODS (MA957, PM2000, EUROFER, K3, etc.) irradiated at different temp, dpa and dose rates
- Studies of synergism H/He, combination (validation) of recent theoretical models.

Recent scientific events

JRC
EUROPEAN COMMISSION

Institute for Energy

IAEA

Joint EC - IAEA Topical Meeting on:

(F1-TR-37435)

Development of new structural materials for advanced fission and fusion reactor systems

hosted by

FUSION FOR ENERGY

ICFRM-14
Sapporo 2009

IAEA
International Atomic Energy Agency
Atoms For Peace

INFORMATION SHEET

ICFRM-14 Satellite meeting in cooperation with the IAEA on

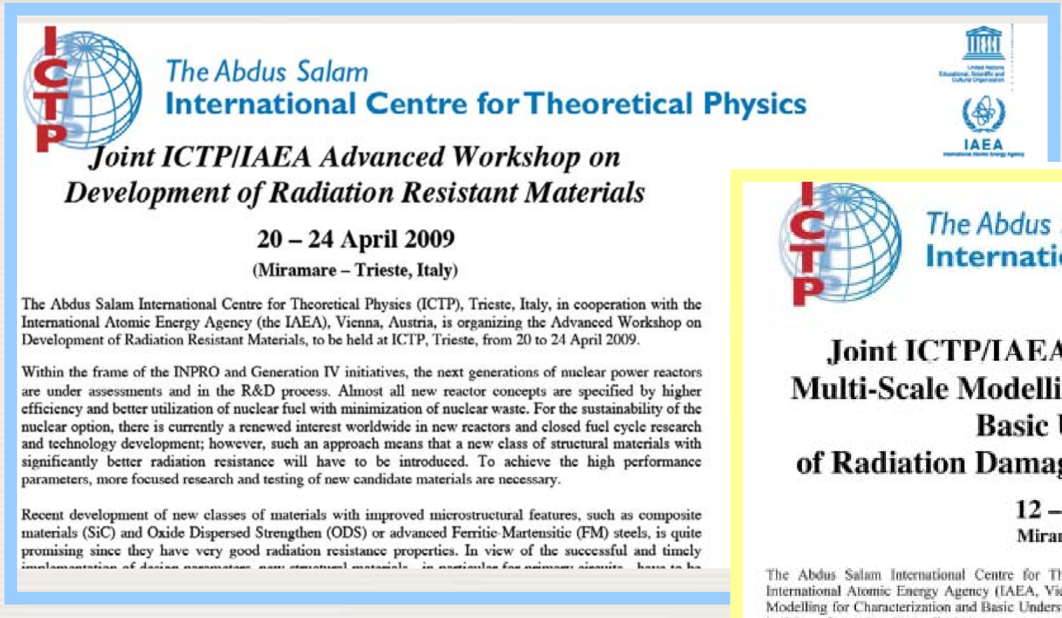
Cross-cutting issues of structural materials for fusion and fission applications

14th International Conference on
Fusion Reactor Materials
(ICFRM-14)

10 - 11 September 2009

http://meeting.iaea.org/

Education & training activities



The Abdus Salam
International Centre for Theoretical Physics

Joint ICTP/IAEA Advanced Workshop on
Development of Radiation Resistant Materials

20 – 24 April 2009

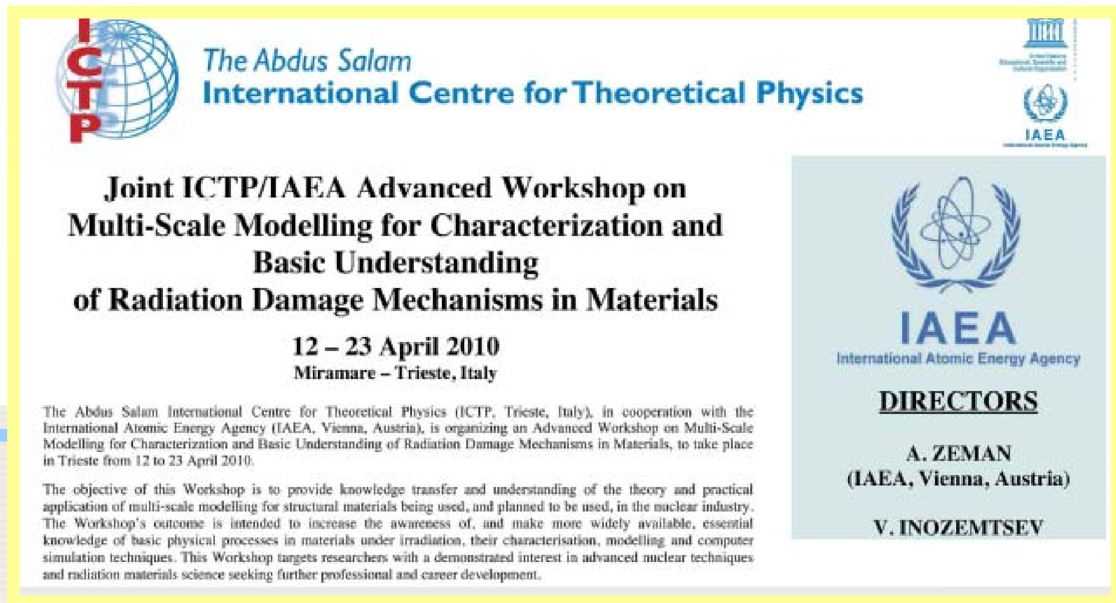
(Miramare – Trieste, Italy)

The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, in cooperation with the International Atomic Energy Agency (the IAEA), Vienna, Austria, is organizing the Advanced Workshop on Development of Radiation Resistant Materials, to be held at ICTP, Trieste, from 20 to 24 April 2009.

Within the frame of the INPRO and Generation IV initiatives, the next generations of nuclear power reactors are under assessments and in the R&D process. Almost all new reactor concepts are specified by higher efficiency and better utilization of nuclear fuel with minimization of nuclear waste. For the sustainability of the nuclear option, there is currently a renewed interest worldwide in new reactors and closed fuel cycle research and technology development; however, such an approach means that a new class of structural materials with significantly better radiation resistance will have to be introduced. To achieve the high performance parameters, more focused research and testing of new candidate materials are necessary.

Recent development of new classes of materials with improved microstructural features, such as composite materials (SiC) and Oxide Dispersed Strengthen (ODS) or advanced Ferritic-Martensitic (FM) steels, is quite promising since they have very good radiation resistance properties. In view of the successful and timely

Open to IAEA & UNESCO Member States, see



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12 – 23 April 2010
Miramare – Trieste, Italy

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The objective of this Workshop is to provide knowledge transfer and understanding of the theory and practical application of multi-scale modelling for structural materials being used, and planned to be used, in the nuclear industry. The Workshop's outcome is intended to increase the awareness of, and make more widely available, essential knowledge of basic physical processes in materials under irradiation, their characterisation, modelling and computer simulation techniques. This Workshop targets researchers with a demonstrated interest in advanced nuclear techniques and radiation materials science seeking further professional and career development.

IAEA
International Atomic Energy Agency

DIRECTORS

A. ZEMAN
(IAEA, Vienna, Austria)

V. INOZEMTSEV

More info: www.ictp.it

- Support of international and regional education and trainings
- Cooperation with ICTP and other collaborating centres (ANSTO, RID, Elletra, etc.)

Recent R&D issues

- Roadmaps on IR, national priorities (GIF portfolio: SFR, LFR, GCR, MSR, VHTR, SCWR).
- Consideration: Design - Coolant - Material (pathway)
- Structural materials : critical issues for several concepts
- Basic research - screening of candidate materials -confirmation - qualification procedure, most of the steels developed 70-80 are not suitable (P91, T91, MA956, 304, 316)
- Characterize the operating conditions of critical replaceable and non-replaceable components (EOL dose, operational temperature and transition regimes, neutron flux, chemical compatibility with coolant, mechanical stress, and design lifetime).
- Pre-selection of candidate materials, consideration of research outputs in fusion in order to analyse long-term behaviour

GEN-IV material development

GIF R&D Outlook for Generation IV Nuclear Energy Systems (2009)

- VHTR unique components needed, including the RPV, intermediate heat exchangers, and Brayton cycle turbo-machinery. RPV size and thickness being larger than modern boiling water reactor vessels.
- SFR development of advanced structural materials may allow further design simplification and/or improved reliability (e.g., low thermal expansion structures and greater resistance to fatigue cracking). These new structural materials need to be qualified, and the potential for higher temperature operation evaluated.
- SCWR development of materials and components will build on (1) evaluation of candidate materials with regard to corrosion and stress corrosion cracking, strength, embrittlement and creep resistance, and dimensional and micro-structural stability; (2) the potential for water chemistry control to minimize impacts as well as rates of deposition on fuel cladding and turbine blades; and (3) measurement of performance data in an in-pile loop.

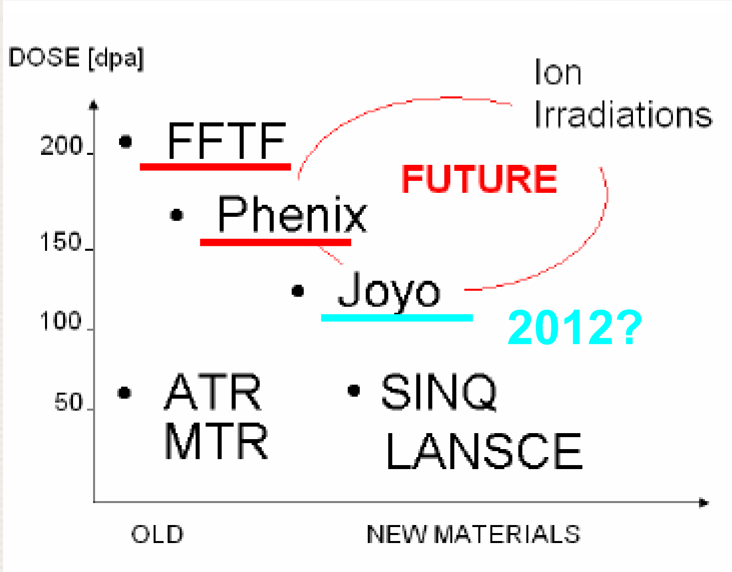
GEN-IV material development

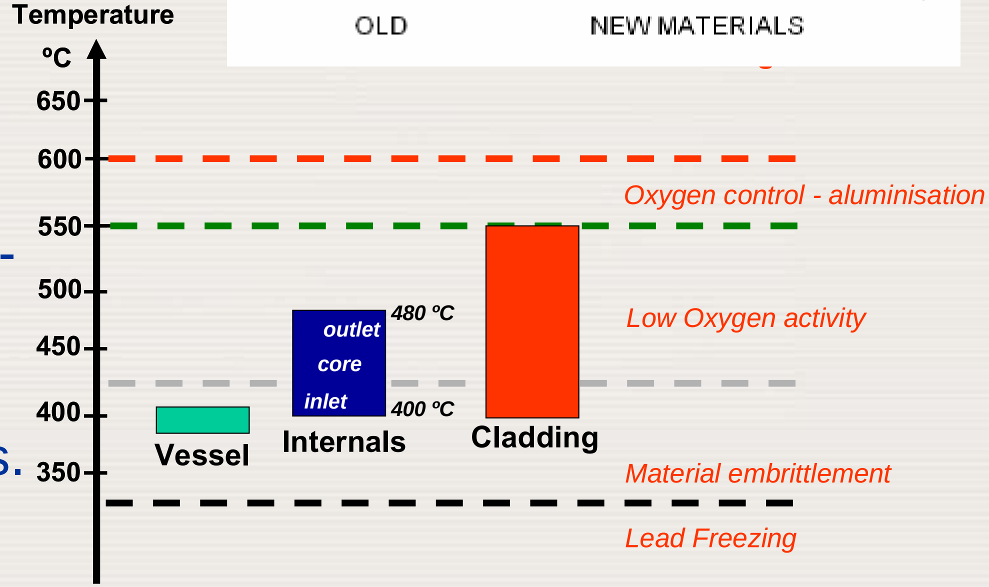
- GFR many of the structural materials and methods could be adopted from VHTR, including RPV, hot duct materials, and design approach. RPV is thick martensitic Cr-steel structure, ensuring negligible creep at operating temperature.
- LFR corrosion of structural materials in Pb key issue, corrosion of steels depends on the T and (O). In addition, surface oxidation and erosion to dissolution of the structural steel (oxidation rate, flow velocity, temperature, and stress conditions). FM and AS compatibility with Pb has been extensively studied and it has been demonstrated that generally below 450°C!, with an adequate oxygen activity in the liquid metal, both types of steels build up an oxide layer which behaves as a corrosion barrier, above 500°C?, corrosion protection through the oxide barrier appears to fail (e.g. T91 and AISI 316).
- MSR main steps are the experimental validation of SM behaviour (mechanical properties, corrosion), like Ni-based alloys including increased T, and the investigation of fission product deposition on structures and embrittlement.

R&D pathway - critical issues

Debarberis et al., IAEA-ICTP Advance Workshop on Development of Radiation resistant materials, ICTP Trieste, 20-24 April 2009

- Available materials - only dedicated data exist, limited information at high dose, temperatures, realistic conditions
- Materials not optimised (T91, MA956, HT9)
- New evolutionary materials (RAFM-ODS, Si- Al-enhanced, etc.) to be tested (irradiated), however there is lack of testing facilities (MTR fast spectrum)
- Medium doses achievable (BOR-60, ~ 20 dpa/y)
- Ion-irradiations for high dose (indication), difficult bulk analysis.





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Objectives: up-to-date information on basic theories and computation tools which are needed for modelling of physical properties and radiation effects at different levels in the multi-scale approach.

Specific topics:

- Theories applicable for characterisation of properties at various time and dimensional scales
- Degradation mechanisms of material microstructures and properties
- Physical models implemented into computer codes for material properties and simulation of behaviour under irradiation
- Tools for experimental validation and benchmarking of multi-scale models
- Application of multi-scale modelling approach to studies of radiation effects in selected materials and model alloys

Workshop details

Participation: 40 attendees / 27 countries, more than 160 applic.

Program: 48 presentations will be given by 14 senior experts.

Syllabus: available electronically at ICTP web page.

Posters: 32 posters to be displayed during 3 sessions from 12 to 14 April, evaluation will be done and best 3 authors will get timeslot for oral presentations.

Technical tour: visit of ELLETRA synchrotron facility (IAEA CC) planned on 15 April.

Workshop questionnaire: feedback regarding WS organisation issues.

Thank you for your attention

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