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Accelerator Simulation and Theoretical Modeling of Radiation Effects (SMoRE)

Report of the Technical Meeting

International Atomic Energy Agency

hosted by
NSC - Kharkov Institute of Physics and Technology
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Contents

1. Introduction

Materials properties can be strongly affected by irradiation, and therefore the behavior of materials under irradiation has been studied for more than 50 years. However not all scientific and technological aspects have been fully understood, with further research still necessary. In particular, there is a lack of information for new and improved core materials irradiated at very high neutron doses. This is for two principle reasons:

1) Experimental facilities with the appropriate neutron spectrum are either not accessible or are not currently available.
2) Irradiation with neutrons to the required fluences would take decades to accomplish.

In general, the role of the structural materials for fission and fusion reactors is to retain functionality. These materials must maintain the integrity of individual components, such as fuel rods and assemblies where the release of radioactivity to the coolant and environment must be prevented, during both normal and transient operations. Materials were originally chosen on the basis of their as-fabricated properties. However there is an inevitable evolution of properties, induced by radiation, with most changes being detrimental in nature. The important point, on the other hand, is that these degradations can be mitigated or delayed, through material modifications and attention to the details of the radiation environment.

The high irradiation doses and temperatures planned for advanced fission and future fusion reactors will most certainly require the development of new improved materials. The cost of material testing with neutron irradiation for these advanced nuclear systems is continuously increasing, while availability of test reactors is steadily decreasing. Currently the cycle of necessary examinations of an improved material for industrial employment in existing reactors requires 20 or more years. These factors make it almost impossible to conduct direct reactor experiments for the development of new materials for advanced nuclear systems. The rational alternative is then the development of experimental simulation, with particle irradiations other than neutrons, together with theory based computational simulation tools. Such models have the objective of making science based predictions of material behavior, under anticipated operational conditions of a fission or fusion neutron environment. It has been frequently demonstrated that charged particle simulation experiments, backed by theoretical modelling of radiation effects, can be used effectively to reduce both the cost and duration of the R&D stage (directly), testing (partly) and industrialization and licensing (progressively, as far as proven knowledge and experience are accumulated). Since accelerators play a very important role in technological development and industrial applications, furthering accelerator studies coupled with modeling shows huge potential. The opportunity to increase our fundamental understanding of radiation damage in high dose materials; validation, verification; extended time and length scales of complex material modeling; and a more effective and integrated use of novel characterization techniques, to take full advantage of their complementary applications.

2. Objectives of the meeting

The overall objective of the Technical Meeting was to provide a forum to exchange ideas and information through scientific presentations and brainstorming discussions.

The aim of the meeting was to demonstrate how experimental accelerator simulation methods and theoretical modeling tools could be applied to investigate irradiation phenomena, which degrade physical and mechanical properties and induce dimensional changes.

The following particular objectives have been specified:

(a) Gaining a better understanding of radiation effects and mechanisms of material damage and the basic physics of accelerator irradiation under specific conditions.
(b) Presenting the latest developments in understanding radiation effects and recent theoretical modeling.
(c) Contributing to the international consensus in the developmental efforts on advanced structural materials and nuclear fuel cycle technologies.
(d) Fostering advanced or innovative technologies by promotion of information exchange, collaboration, and networking.

The specific objective of the IAEA Coordinated Research Project on "Accelerator Simulation and Theoretical Modeling of Radiation Effects (SMoRE)" has also been discussed. Further sharing of information and experience in the application of accelerator irradiation for fission reactors, as well as in other nuclear concepts such as fusion and spallation systems, is a key step forward. A general objective which was discussed was the methodologies that will bridge the micro- to macroscopic behavior of materials through modeling validated by specific well chosen experiments.

The TM was particularly focused on the specific applications of accelerators and theoretical modeling, together with integration issues.

(a) Advancement of theoretical models of the fundamentals of radiation damage, with respect to core structural materials and high dose nuclear applications through comparison and experimental verification of theoretical and computational models.
(b) Application of advanced characterization techniques down to the atomic level for materials analysis, in combination with ion irradiation experiments.
(c) Specific ion irradiation experiments to understand flux, spectra and ion effects on damage production and property evolution.

The output of the meeting is presented in the form of the meeting summary report from presentations and working groups findings and recommendations. The document reflects the priority and future needs of participants in the field of accelerator simulation and theoretical modeling of radiation effects.

3. Summary of presentations

The IAEA scientific secretaries of the meeting, Mr. A. Zeman (Physics Section, Division of Physical and Chemical Sciences, Department of Nuclear Sciences and Applications) and Mr. V. Inozemtsev (Nuclear Fuel Cycle and Materials Section, Division of Nuclear Fuel Cycle and Waste Technologies, Department of Nuclear Energy) welcomed all participants on behalf of the IAEA. They presented the general objectives of the Technical Meeting (TM) and thanked the local organizers for hosting the meeting at the Kharkov Institute of Physical Technology (KIPT). After a brief IAEA introduction, the Chair of the Meeting, and the Director General of the KIPT, Academician, I. Neklyudov, greeted all participants, informed them about the history and present activities of the host Institute, and opened the TM.

In total 26 experts and researchers from 10 different countries attended the Technical Meeting and 15 scientific presentations were given.

The agenda of the meeting was accepted and three sessions of presentations were held on 9-11 June followed by a Technical tour to the KIPT facilities on 12 June and a Summary Session on 13 June 2008. On the evenings of 9 and 11 June there were Working Group discussions of concerns, issues, wishes, and expectations from the planned IAEA CRP SMoRE.

Session 1 (9 June), Session Chair - Prof. V. Voyevodin (KIPT)

Paper 1

Mr. V. Voyevodin (KIPT) (Kharkov Institute of Physics and Technology, Kharkov Ukraine) gave a talk on “Accelerator Simulation of Structure-Phase Evolution and Radiation Resistance of Materials for Nuclear Reactors”. He pointed out that there is a need to continue research and development of structural materials for existing and developed nuclear facilities. Prof. Voyevodin emphasized that the problem of developing materials to operate in unique conditions of irradiation, and in evaluating their radiation resistance, can be solved through the use of existing irradiation facilities. This would allow both the determination of the mechanisms of radiation damage and also the selection of materials with high radiation resistance. Moreover, the trend for available neutron irradiation possibilities has been strongly decreased due to the shut down of many nuclear facilities. Therefore, accelerators can be used very effectively as an alternative. The main advantage is not only the obtaining of rapid results, but the possibility of understanding basic mechanisms and of separately investigating the influence on irradiation damage of many different variables. Selecting particular particles and energies allows one to study factors of importance in reactor irradiations. It was shown that differences in the process of nucleation and the evolution of dislocation and void structures exist between cascade (heavy ions) and non-cascade (HVEM) cases. Accelerator experiments are also employed in creating temperature and dose dependence studies of the evolution of dislocation ensembles, void structures, and precipitates. Such studies were shown to be able to provide the critical data for models of commercial materials. It was demonstrated that accelerator experiments involving structural changes, phase transformations, and void swelling are particularly productive because they allow one to methodically investigate the influence of different irradiation factors. Many experiments are understood with regards to their role in studying structural phase evolution, the influence of crystal lattice, and gaseous impurities etc. The consequences of different alloying elements in irradiation experiments of cladding for fuel elements was also shown.

In the conclusions of this paper it is noted that there is need for further development of accelerator-based experiments and irradiation programs which are especially desirable in the elucidation of fundamental processes; the R&D of advanced materials for fast reactors (swelling and embrittlement), life extension of reactors, RPV steels (dpa rate, minor alloying elements), and RVI (low temperature swelling and embrittlement) as well as synergetic effects of helium and hydrogen in fusion and spallation systems.

Paper 2

Mr. V. Storizhko (Institute of Applied Physics, National Academy of Sciences of Ukraine**),** presented "IAP accelerator based facility for simulation and studies of radiation induced defects in materials". Mr. Storizhko overviewed the key research activities at the Institute of Applied Physics of the National Academy of Sciences of Ukraine. He presented recent developments of electrostatic accelerators for the simulation of the radiation damage and 3D characterization of the reactor materials structure and composition. The IAP laboratories are well-equipped with different instrumentations and support services for the investigation of all aspects of the composition, microstructure and defect properties of reactor materials. 2MV electrostatic accelerator is a facility dedicated to ion microanalysis of materials from atomic to microscopic levels. Academician Storizkko presented the experimental capabilities and instrumentations, in particular: Particle Induced X-ray Emission, Rutherford Back Scattering, Rutherford Forward Scattering, Nuclear Reaction Analysis, Scanning Ion Microanalysis, Ion Luminescence Spectroscopy. Different analytical instruments are also available: Laser Mass-Spectrometer with position sensitive detector, Mass Spectrometer with soft ionization, Atomic Absorption Spectrometer and some others. The laboratory for ion implantation research is capable of performing high dose ion implantation and modification of surface layers of solid samples. Presently this team is busy with the design and construction of a high-current (I~50mA) H+/H- ion source and a cluster source. The commissioning of the AMS-4130 Accelerator Mass Spectrometer purchased from the HVEE company and intended for isotope mass analysis took place. Planned schedule for period 2009-2010 includes the construction of another electrostatic accelerator to produce electron/positron/ion beams of energies approaching 6MV which are to be used in both microanalyses and simulations of radiation damage at ultra-low temperatures. Mr. Storizhko pointed out the need for continuous research programs and developments for new analytical accelerator based facilities; with nanometer spatial resolution for reactor material characterization. It should be combined with first-principles simulation studies, taking into account the magnetic effects of ferromagnetic alloys. And finally, more precise experimental data on radiation effects are needed to validate the existing first-principles approach (the international program of reference materials).

Paper 3

Mr. Y. Konobeev (State Scientific Center of Russian Federation – Institute for Physics and Power Engineering named after A.I. Leipunsky, Obninsk, Russia), presented a talk on the "Center of Accelerator Simulation and Theoretical Modeling of Irradiation phenomena in SSC RF IPPE". Professor Konobeev overviewed the situation on ion irradiation techniques and applications of accelerators as a useful tool for studying void swelling, radiation-induced changes of phase composition and microstructure in metallic alloys. The majority of physical trends found out by ion irradiation testing have been confirmed in subsequent reactor experiments. Experimental data from accelerator simulations have appeared important for developing models of irradiation phenomena. Mr. Konobeev explained that ion irradiation in accelerators and theoretical modelling should be used to investigate radiation-induced segregation in alloys. This phenomenon may affect many irradiation phenomena, such as void swelling, changes in phase composition etc. The irradiation by heavy ions of 5-10 MeV energy will be especially informative.

Paper 4

Mr. A. Ryazanov (Russian Research Center, Kurchatov Institute, Moscow Russian Federation) presented the talk on "Using of charge particle accelerators for investigations of physical mechanisms of radiation resistance of fission and fusion structural materials". In particular, the radiation resistance of fission and fusion structural materials is determined by such physical phenomena as radiation swelling and creep, radiation hardening, helium and hydrogen embrittlement. However, all these important processes depend on microstructural changes in irradiated materials, which are characterized by generation rate of point defects, cascade efficiency, irradiation temperature and dose dependence. All these values can be obtained and reproduced at different temperatures in accelerators of charged particles. Professor Ryazanov pointed out that the experimental tests in atomic reactors are very expensive and take a long time. Therefore the irradiation of these materials by fast charged particles on accelerates reveals experimental data concerning the radiation resistance of structural materials; that is, during a short time, thus without high radioactivity levels on irradiated samples. Each physical phenomenon can be studied at fixed temperatures and irradiation doses in displaced atoms. The review of the latest experimental methods and results in this area are presented in this report. The new experimental methods and results for the analysis of microstructural changes in irradiated materials (including X-ray methods on synchrotron source and Transmission Electron Microscopy) will be very helpful in a more detailed investigation. He emphasized that the effect of helium atom saturation of ferritic – martensitic steels (ODS) on accelerators with alpha-particle energies up to 30MeV are needed. Furthermore, post treatment mechanical and TEM tests will be very effective for understanding the behaviour of these materials at high appm He levels. Mr. Ryazanove summarized his presentation briefly. He pointed out that the further development of theoretical models for investigating He+H effects, together with radiation damage accumulation, is very important. Such an approach can help to further understanding of experimental results on triple type ion irradiation in metallic alloys.

Paper 5

Mr. G. Tolstolutskaya (National Science Center, Kharkov Institute of Physics and Technology); "Retention and Features of Deuterium Detrapping from Radiation-Induced Damage in Steels". The presentation provided an overview of the accelerators and ion beam analysis techniques, used for simulating displacement damage and performing detailed studies of distribution profiles of damage and impurity gas atoms (especially helium and hydrogen) under a wide range of irradiation doses and energies. Helium and hydrogen are known to play an important role in the evolution of damage microstructure. This may affect the mechanical properties and cracking behavior of structural materials. Ms. Tolstolutskaya presented the results obtained for 18Cr10NiTi stainless steel. They show that ion implanted deuterium is weakly trapped by defects produced in 5 keV D+ displacement cascades. The effective trapping temperature interval is 300-600K. By comparing experimental curves with data based on models of hydrogen diffusion in the presence of defects, it was established that ion implanted deuterium is trapped by radiation vacancies complexes. It was shown that the presence of surface passive film considerably displaces the gas release intervals to high temperatures and, on several orders of magnitude, reduces the deuterium surface recombination coefficient. Influence of atmospheric oxygen on surface layers of Ti-containing stainless steels results in formation of strong hydrogen traps in the vicinity of the film-metal interface. However, the characteristics of trapping (e.g. the temperature range of retention of hydrogen isotopes in traps, via prior He implantation) depends on the concentration of implanted helium and on the type of developed defects. Formation of helium bubbles in 18Cr10NiTi steel causes an increase of retained deuterium by one order of magnitude in a wider range of temperatures, 500-1000K.

Implanted helium and heavy ion induced damage on deuterium trapping in austenitic and ferritic/martensitic steels was studied. Energetic heavy ion irradiation (1.4 MeV Ar+) was used to model defect cluster formation under displacement cascade conditions so as to simulate fusion reactor environments. It was found that retention of hydrogen and deuterium is strongly enhanced by the presence of helium (especially at large He amounts) and argon atoms.

A recommendation was made to continue in the investigation and research of synergistic effects of helium and hydrogen for defect evaluation; vacancy trapping and void nucleation associated with He and H gases in the presence of induced simultaneous damage. Moreover, new experimental facilities have to be promoted in the future, in particular, for triple-ion irradiation (dpa damage, plus helium, and hydrogen). This utilises ion beam techniques for (a) simulating displacement damage and (b) detailed investigations of distribution profiles of damage and impurity atoms (especially helium and hydrogen) under targets irradiated over a wide range of doses and energies.

Session 2 (10 June), Session Chair – Prof. A. Ryazanov (RRC-KI)

Six reports have been presented on this section of IAEA TM 34567 SmoRE concerning theoretical modelling and experimental investigations on the effect of irradiation on different types of materials.

Paper 1

Mr. G. Monnet (EDF – R&D, MMC, France) gave a first report on "Dislocation Dynamics study of low and high temperature mechanical behavior of ferritic steels". The theoretical modelling of dislocation motion in ferritic steel has been presented. It is based on the modern theoretical models for describing glide dislocations for the screw and edge dislocations.

Ferritic steels are known to undergo the ductile to fragile transition at low temperature. The physical origin involves slip activity and dislocation mobility. Dislocation Dynamics (DD) simulations were used to predict the collective behavior of dislocations in Reactor Pressure Vessel (RPV) steel. The multiscale-simulation framework used in this study allows us to account for the evolution of physical features involved in plastic deformation as a function of temperature. The dislocation mobility, which constitutes the only input parameter of the simulation, is estimated from molecular dynamics simulations and mechanical tests performed on iron single crystals.

It was shown that strengthening mechanisms are strongly affected by temperature through thermal activation processes. On the one hand, the strength of dislocation-dislocation interactions reduces with decreasing temperature. The reason is associated to the loss of mobility of screw dislocations, inhibiting dislocation curvature, which is necessary to enable junction formation. Results show clearly that strain hardening should decrease with decreasing temperature. On the other hand, the carbide – dislocation interaction is also found to decrease at low temperature, due to the large mobility of non-screw dislocations.

The main suggestion for future research in this topic is to include further numerical calculations for the climb of dislocations in the model. This must take into account radiation damage accumulation in the matrix of irradiated materials.

Paper 2

Mr M. Lazarev (NSC Kharkov Institute of Physics and Technology, Ukraine) gave a talk on the "Molecular dynamics simulation of track development in a model NiAl alloy". The theoretical model of track formation in memory alloy NiAl has been developed based on the "Thermal Spike Model".

At the high-energy regime with ion energy E_i > 100 MeV, the track evolution in a martensite phase results in the melting of its core. Subsequent cooling leads to the formation of an amorphous zone in the central part of the track and considerable austenite region can be found around the periphery of track. Various phase transformations are induced in the track range: crystal-liquid-glass-crystal, martensitic, compositional order-disorder transformations. These transformations occur at length scales of ~10 *nm* from track centre and at time scales of up to 1*ns*. In order to get more insight in these phenomena we performed molecular dynamic simulations of phase transformations in a model NiAl alloy.

The talk starts with a study of the thermodynamic and kinetic properties of the model NiAl alloy [1,2]. To distinguish structural changes during phase transformations, usually radial distribution functions are calculated which describe the structure - on average. For detailed investigations of the structure development, a new approach of local order parameter of alloy undergoing structural rearrangements is used. This method is based on combination of Voronoy tessellations and the common-neighbor analysis. Also, the basis of an analysis of local chemical order changes is discussed.

The development of new phases around a swift ion track in NiAl alloy is simulated. We use two basic concepts. The first is a thermal spike model for evolution of energy transfer from swift ion to electronic system under ballistic collisions. For the atomic system we apply a molecular dynamics method where the electronic system is used as an external thermal bath. The central part of the track appears to be highly disordered and has a tendency to transform into amorphous state. The outer part indicates the formation of heterogeneously distributed austenite B2 ordered regions.

A suggestion for further improvement is to include the "Coulomb explosion model" in the numerical modelling.

Paper 3

Mr. D.O.Krarchenko (National Academy of Sciences of Ukraine) presented a report: on "Monte-Carlo modeling for unstable particle ensembles in system with thermal fluctuations". The theoretical modelling of phase transitions based on microscopic models of unstable metallic systems has been developed.

Prototype models demonstrating the formation of super lattices of particle densities as a result of their interactions were considered. One assumes that unstable particles are generated and degenerated in the process of system evolution (internodal atoms and vacancies; excitons, intermediate particles in isomerization reactions, etc.). The existence of these particles is due to the influence of external sources such as the intensive irradiation of crystals; transmutation processes, etc. Therefore, a system representing the above ensembles is considered to be in nonequilibrium. If the particle density is large, then the interaction processes start to play a crucial role. It leads to a new phase appearance caused by collective effects. Considering a system under real conditions, one has to take into account fluctuations caused by particle interactions and diffusion flux noise.

In this work it was presented the results of Monte-Carlo simulations were presented. Mean-field approaches were also shown, which illustrate that systems of unstable particles belonging to *A* and *B* classes (with no conserved and conserved dynamics, respectively) can undergo phase transitions induced by thermal fluctuation with spatial patterns (super lattices) formation. It was found out that if the mobility of particles depends on their density, then quasi equilibrium phase transitions of reentrant types are observed. In the model *A*, with an increase in the thermal fluctuations intensity, the system undergoes the reentrant phase transitions: an order parameter reduced to the averaged local magnetization value increases, and then decreases with growth in fluctuation intensity. For the model *B*, the same situation is observed: an increase in the noise intensity leads to the reentrant behavior of the order parameter reduced to the second moment of stochastic concentration field. Here we generalize the domain growth law, varying the parameter that controls the field-dependent mobility. Our analytical results are in good correspondence with Monte-Carlo simulations and coincide with well-known literature data. At last, we have considered a complicated model including two above ones: generation/degeneration of unstable particles and their interactions resulting phase separation. Here we study stationary patterns appeared during the system evolution. We verify our analytical predictions using computer simulations.

The derived formalism can be used to describe (a) the formation of super lattices during the processes of generation and degeneration of unstable particles and (b) their interactions at large densities under the intensive irradiation of crystals.

We have a strong recommendation to include radiation damage effects in further considerations.

Paper 4

Mr M.J. Fluss (Lawrence Livermore National Laboratory, USA) presented in the next report "Experimental Determination of Metal Fuel Point Defect Parameters". The experimental data for changes of resistivity and magnetic properties in self irradiated and proton irradiated Pu and Pu (Ga) materials have been presented.

Nuclear metallic fuels are one of many options for advanced nuclear fuel cycles because they provide dimensional stability, mechanical integrity, thermal efficiency, and irradiation resistance. The associated pyro-processing is technically relevant to concerns about proliferation and diversion of special nuclear materials. In this presentation we will discuss recent success that we have had in studying isochronal annealing of damage cascades in Pu and Pu(Ga) arising from the self-decay of Pu. The annealing characteristics of non-interacting point defect populations produced by ion accelerator irradiation are also investigated. Comparisons of the annealing properties of these two populations of defects (arising from very different source terms) are enlightening. They point to complex defect and mass transport properties in the plutonium specimens, which are only now starting to be understood due to many follow-on studies. More importantly however, the success of these measurements points the way to obtaining important mass transport parameters. These could be used for comparison with theoretical predictions, or for direct use in existing and future material modelling of radiation effects in nuclear metallic fuels. The way forward on such measurements, together with the required theory and modelling will be discussed.

Paper 5

Mr. L.Gamez (Instituto de Fusion Nuclear, Spain) reported on “Kinetic Monte Carlo simulations of Helium implantation and desorption from Nickel”. The experimental data concerning helium desorption mechanisms in helium implanted nickel with different energies of helium ions were presented.

It is known that the presence of impurities such as He can enhance the production of bubbles and voids in metals, particularly in austenitic steels, giving rise to swelling and detrimental effects in the mechanical properties of these materials. In this work, the particular case of Ni is studied using kinetic Monte Carlo methods with input from molecular dynamics calculations and first principles ab initio data available in the literature. Simulations are performed to study the implantation of He in Ni under different conditions of irradiation dose and temperature. The desorption of He during isochronal and isothermal annealing is obtained and results were compared with available experimental data. From these calculations, relevant mechanisms of He diffusion and He-V complex stabilities were revealed that provide insight on the initial stages of bubble and void nucleation in f.c.c. metals. Results were discussed and compared to other calculations in b.c.c. metals, in particular Fe.

The obtained results for the helium desorption should give the real values of energy migrations for interstitial and substitution positions of helium atoms in the matrix of implanted materials.

Paper 6

Mr. D.Terentyev (SCK-CEN, Belgium) presented “Radiation damage in Fe-Cr alloys for nuclear applications”. A review of the effect of irradiation on Fe-Cr alloys with the different composition of Cr atoms is given.

High-Cr ferritic/martensitic steels (containing 7-14%Cr) were being considered as structural materials for a large number of future nuclear applications, from fusion to fission accelerator-driven systems and GenIV reactors. Understanding the basic mechanisms governing their behaviour under neutron irradiation is therefore highly important.

The performance of high-Cr steels and their base (Fe-Cr alloys), under irradiation, is largely determined by the Cr content. For instance, a well-known local minimum in the ductile-brittle transition temperature shift after irradiation has been identified for steels and binary alloys containing ~9%Cr. The addition of Cr also significantly reduces void swelling, reaching a minimum at ~5 ÷12% Cr, depending on temperature and dose. The origin of these and other Cr-dependent effects is most likely to be attributed to the magnetic nature of high-Cr steels, as a consequence of which Cr has an extraordinary high solubility limit in Fe (~10%). Below it, Cr atoms tend to order; above, they tend to precipitate. Such dual behaviour apparently has an influence also on the microstructure evolution and consequently on the response of the materials to mechanical load. Interestingly, the best performance is usually observed for steels and Fe-Cr alloys with Cr composition close to 10%.

The construction of a whole modelling framework was required to provide at least some indicative interpretation for these experimental findings. This involved *ab initio* calculations and the development of new formalisms for interatomic potentials for large-scale atomistic simulations. With these, primary damage, defect migration and dislocation-defect interactions were studied using atomistic approaches, which also now allow the complex thermodynamics of the Fe-Cr system to be reproduced. In parallel, oriented-oriented experiments on Fe-Cr alloys, e.g. those irradiated in the BR2 reactor (SCK•CEN, Mol, Belgium), have been performed and helped, when combined to the information from modelling, to understand the mechanisms playing a role in radiation damage versus Cr content.

Here an overview of part of the effort made to model radiation damage in Fe-Cr alloys was presented. Some recent results are highlighted that provide a key for interpreting existing and so far unexplained experimental results. In turn, experimental results provide a framework for further investigation and validation of theoretical models.

The suggestion for the further investigations: try to give the physical explanation of the effect of different concentrations of Cr atoms on the radiation resistance of Fe-Cr alloys.

Session 3 (11 June), Session Chair – Dr. M. J. Fluss (LLNL)

Paper 1

Mr. V. Kumar (Department of Physics, University of Rajasthan, Jaipur, India) presented a paper titled, “A Study of Accelerator Driven Sub critical System- Material Using the Cascade Code”, with co-authors, H. Kumawat and C. Bhatia. The paper provided a brief history of the development of the CASCADE code, its origin with V. S. Barashenkov and the participation of Indian scientists in its extension and futher development. A representative description of the Benchmarking of the Reaction cross section and validation of code was provided followed by cross-section results for the production of isotopes and neutrons from various ADS materials. The paper outlined the current status of (n,xn) reactions. A number of conclusions were reached in the presentation.

Reaction cross sections are well predicted by the CASCADE, code. More precise neutron-cross sections from accelerators are required. Production cross sections are closely predicted (but all are not tested). Monitor reaction cross sections that are very useful on accelerators, are obtained from simulation by the CASCADE code. Even-odd effects are present in both experimental data and the CASCADE code; it is recommended that this should be theoretically studied. The (n, xn) contribution in neutron-production is different in different nuclei. It can be as much as 90 % at certain energies and it varies with the target. Study of (n, xn) reactions is demonstrated to help in the understanding of the fuel combinations for ADS in a more logical manner. Current results hint towards an uneven heat distribution in the target system. For the radiation damage study for ADS there is need of developing a code for the transport of neutrons and isotopes through ADS materials. This will require new data libraries specific to this problem.

Paper 2

Mr. S.Zhu (China Institute of Atomic Energy, Beijing, China) presented a paper titled, “Heavy Ion Irradiation Simulation of High Dose Irradiation and Induced Radiation Damage in Materials”. The paper presented a brief history and description of ion irradiation facilities at China Institute of Atomic Energy (CIAE) and the available post irradiation examination capabilities using positron annihilation life-time spectroscopy (PALS). Four related ion-beam radiation damage and PALS analysis topics were described: 1) dependence of radiation damage on irradiation temperature and dose in Modified 316L SS (MSS), 2) comparison of radiation damage in stainless steels and tungsten, 3) dose dependence of radiation damage in W and Ta and, 4) comparison of radiation damage in three stainless steels, a low activation Chinese developed steel (CLAM), F82H, and T91.

While the studies provided interesting qualitative results, they lacked detailed explanations based on radiation damage theory. It was not clear how inter comparisons were normalized, one to the other, either across different materials or different ions and ion energies. During questions the relationship between dpa depth profiles and the positron stopping profile were questioned but were not clarified. The facilities at CIAE are impressive and offer great potential when more well controlled experiments and complimentary post irradiation techniques are employed. Conclusions reached by Dr. Zhu were: that HIIS makes it possible to investigate RD induced by high dose neutron and/or proton irradiations in lab in a short time period, something that all would agree with, that microscopic analysis of RD is very useful but in discussion complimentary techniques are required, and inter comparison studies are capable of providing useful material selection information once a more quantitative interpretation of data can be achieved. Of particular note is the apparent good performance of the CLAM steel relative to other well-known steels.

Paper 3

Mr. V. Kršjak, (Department of Nuclear Physics and Technolog,y Slovak University of Technology), presented a paper titled "Ion Implantation Induced Defects in Fe-Cr Alloys Studied by Conventional Positron Annihilation Lifetime Spectroscopy Slow Positron Beam", with co-authors Stanislav Sojak, and Vladimír Slugeň. The presentation gave an exposition on the fundamentals of ion beam radiation damage and positron annihilation techniques with an emphasis on positron annihilation lifetime spectroscopy (PALS) using conventional sources and positron beams. The topics covered were: 1) experimental approach to study radiation damage, 2) an introduction to positron annihilation spectroscopy, and measuring of the positron lifetime (elementary principles), 3 application of conventional PALS and positron beams in the study of helium implanted Fe-Cr alloys along with a discussion of complementary non-destructive experimental techniques.

It was emphasized that there is no experimental technique, sufficient to describe the complicated behavior of real materials microstructure under radiation treatment. Therefore different techniques need to be combined for this purpose. As an example light ion implantation can be successfully applied as a material degradation tool (the simulation of neutron flux) and created defects can be experimentally studied by various techniques. More specifically was the study of FeCr as a function of Cr concentration. Positron lifetime experiments show that chromium plays an important role in the formation of the microstructure under radiation treatment. In particular, higher chromium content in FeCr alloys leads to a uniform distribution of small defects rather then vacancy defect clustering. Depth profiles of defects in the helium implanted region, obtained with pulsed low energy positron beam (PLEPS) at the Military University in Munich, reflect the helium implantation profiles and show the creation of small vacancy clusters and large voids. These defects cannot be observed by any other technique in a non-destructive way. The work is a very good start on a very important problem related to radiation tolerant steels.

Paper 4

Mr. C.Robertson (CEA, Saclay), presented a paper titled "Plastic Deformation in Ion-Irradiated Austenitic Stainless Steels" with co-authors, Thomas Nogaret, D. Rodney, M. Fivel and Y. Bréchet. The study was inspired by the evolving mechanical properties of reactor pressure vessel, internal structure, austenitic stainless steels during 300-350C neutron irradiation. The approach was carefully outlined. It was emphasized that this was a multi-scale problem, on the mm scale hardening ductility and then softening evolved, on the micro-scale strain localization was evident in clear band formation, and on the nano-scale Frank interstitial loops and dislocation and loop interactions were operative. The specific goal was to rationalize the formation of clear bands.

The approach was a classic example of multi-scale modeling and experiments. TEM was combined with radiation and deformation studies to produce specimens that could be analyzed on the scale of computations. What emerged was a new scenario of clear band formation based on multi-scale modeling. Molecular dynamics revealed the elementary interaction mechanisms describing in detail the dislocation loop interactions through a carefully chosen dislocation dynamics strategy. All modeling was fully experimentally validated.

5. General recommendations

The major findings and recommendations of the Working Groups on Techniques & Experiments (9 June) and Simulations & Modeling (11 June) are as follows:

- "Correlation experiments" approach was suggested. This involves both a traditional round-robin exercise and complimentary irradiation of the same materials by different particles and in different conditions.
- Use of multi-beams and high energy electrons and protons for the simulation of transmutation and synergetic H/He effects was recommended.
- Need of addressing various scales of radiation effects and multi-scale modelling with determination of theoretical bridging, was emphasized.
- Need for advanced qualification of structural and phase states of materials with the application of a broad range of analytical tools, such as 3D nuclear nano-probe techniques, synchrotron sources, some of which have high spatial resolution and/or sensitivity was pointed out.
- Necessity of identifying benchmarks for verification of theoretical models and computational codes was underlined.
- Need to consider all aspects for all irradiation parameters, such as type of particle (neutron, electron, ion), energy spectrum, implantation and temperature profile, dose rate were pointed out.
- Correlation experiments on accessible materials (model alloys e.g. Fe-Cr and Fe-Cr-Ni) for joint studies were recommended.

In addition, more specific issues have been proposed for future studies, as follows:

- Irradiation creep
- Phase transformation and radiation induced segregation on various length scales
- Influence of stress sign and temperature history on swelling
- In-situ experiments
- Role of different impurities and alloying elements in microstructural evolution and embrittlement of core and RPV materials
- Synergy with fusion and ADS materials studies
- Cross sections, energy spectra and other inputs for PKA codes
- Use of small-size (miniaturise) samples and validation process
- Plans for accelerator irradiation testing of neutron irradiated RPV materials were announced by Ukraine and Russia

Difficulties in getting protected commercial materials were mentioned but some opportunities for joint investigations of some Chinese and Russian steels were identified. Necessary amount of material for joint studies is assessed as from 1 to 10 kg depending on scale of investigations.