



The Abdus Salam
**International Centre
for Theoretical Physics**



Joint ICTP-IAEA Workshop on Physics of Radiation Effect and its Simulation for Non-Metallic Condensed Matter

Organizer(s): IAEA: Aliz Simon and Andrej Zeman; Local Organiser: Sandro Scandolo
Trieste - Italy, 13 - 24 August 2012

Final programme

Monday, 13 August 2012 (Room:Adriatico Guest House Kastler Lecture Hall)

- 08:30 - 09:30** (Room: Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1))
--- REGISTRATION ---
- 09:00 - 10:00** --- Coffee served at table nearby registration area ---
- 10:00 - 10:30** **Introduction of the participants**
- 10:30 - 11:30** **Opening of the meeting**
ICTP overview (Sandro Scandolo - ICTP) 30'
Overview of the school; The role of irradiation damage in research and in our everyday life (Aliz Simon - IAEA) 30'
- 11:30 - 13:00** **Ettore Vittone / University of Turin, Italy**
An overview of the electronics properties of semiconductor and insulator materials
The aim of this lecture is to give an introduction to the physical principles underlying the main electronic properties of semiconductor and insulator materials. Particular emphasis will be given on the basic transport mechanisms and on the generation/recombination processes of free carriers in order to provide the fundamental equations governing the electronic behaviour of semiconductor materials. Finally, the principles of operation of basic devices, as pn junction or Schottky diodes, solar cells, Metal-Insulator-Semiconductor (MIS) and transistors (BJT, FET) will be introduced.
- 13:00 - 14:30** --- Lunch Break ---

- 14:30 - 16:00** **Jyrki Raisanen** / *University of Helsinki, Finland*
Fundamentals of ion-matter interactions
The first part of the presentation deals with slowing down of energetic ions in matter. We start with introduction of the basic concepts and parameters. The theoretical formulation for light ion electronic stopping is summarized including, e.g., the concept of stopping number and the related corrections. Comparison with experimental data is surveyed followed by discussion on nuclear stopping. The scaling of proton stopping powers to heavy ion stopping powers by the effective charge formulation is introduced. The topic of energy loss in compounds including Bragg's rule and the Core and Bonds (CAB) model is discussed next. The concepts of straggling and range are discussed to some detail. Various sources providing stopping powers for practical use are listed and the most common associated computer programs are briefly mentioned. The experimental techniques most commonly employed for extracting stopping powers are described. Finally, hadron therapy serves as a topical example where charged particle slowing down plays a clear role. The second part of the presentation deals with radiation effects in solids. The principal effects and the basic terms are briefly discussed along with features associated with defect production by ion bombardment. Common techniques employed for minimizing radiation damage and for crystal recovery are discussed by means of examples.
- 16:00 - 16:30** --- Break ---
- 16:30 - 17:30** **Milko Jaksic** / *Rudjer Boskovic Institute, Zagreb - Croatia*
Irradiation facilities
In order to study and understand changes that occur in materials when exposed to excessive fluences of radiation, different radiation sources and controlled irradiation conditions have to be used. In this review, facilities based on radioisotope sources, accelerators and reactors, as well as principles of their operation for irradiation purpose, will be presented. Discussion and examples on the advantages of electrostatic ion accelerators and in particular use of focused ion beams for studies of radiation damage in materials will be given.
- 18:30 - 20:30** (Room: Adriatico Guest House (Terrace))
Small Reception "Welcome"

Tuesday, 14 August 2012 (Room:Adriatico Guest House Kastler Lecture Hall)

- 09:00 - 10:30** **Gyorgy Vizkelethy** / *Sandia National Laboratory, Albuquerque - United States of America*
Simulation of ion-solid interactions using Binary Collision Approximation
Since computers are becoming larger and faster, the simulation of ion-solid interactions to predict implantation range, ionization profiles, displacement damage, sputtering yield, etc., became an everyday task. In this lecture the different approaches to the simulation will be presented briefly, then the Binary Collision Approximation (BCA) as the mostly used method will be discussed in detail with emphasis on the Marlowe and SRIM computer codes. Examples for the simulation of different phe-nomena will be given.
- 10:30 - 11:00** --- Break ---
- 11:00 - 12:30** **Ettore Vittone** / *University of Turin, Italy*
Theory of the Ion Beam Induced Charge Technique (IBIC)
The acronym IBIC (ion beam induced charge) indicates a scanning microscopy technique which uses MeV ion beams as probes to image the basic electronic properties of semiconductors and to provide exhaustive information on charge transport phenomena occurring in devices, not easily obtainable by other analytical techniques. IBIC is based on the measurement of the charge induced in a given electrode by the motion of charge carriers generated by MeV ions. As such, the modelling of induced charge pulse formation requires a theoretical background involving electrostatics, semiconductor physics and ion-solid interaction This lecture intends to provide the principles of the IBIC technique starting from basic theorems of electrostatics and using the concepts presented in previous lectures. The basic mathematical tools for a correct interpretation of the experimental data will be presented and applied to benchmark experiments to highlight the potential of the techniques.
- 12:30 - 14:00** --- Lunch Break ---

14:30 - 16:00 **György Vizkelethy** / *Sandia National Laboratory, Albuquerque - United States of America*
Hands-on experience with Marlowe and SRIM
In this lecture the actual uses of Marlowe and SRIM will be taught through using these codes. The input parameters and how to interpret and process the output will be shown.

16:00 - 16:30 --- Break ---

16:30 - 17:30 **Poster presentation**

Wednesday, 15 August 2012 (Room:Adriatico Guest House Kastler Lecture Hall)

09:00 - 10:30 **Ettore Vittone** / *University of Turin, Italy*
Modeling of damage in ion irradiated semiconductors
The IBIC technique, expounded in previous lectures, is non destructive if very low fluences of light ions are used. However, if this condition is not fulfilled, a localized damage is induced in the semiconductor, which degrades the performances of the device. Accordingly, ions can be used both to generate recombination or trapping centres and to probe their effects on the transport properties of the material. This lecture intends to illustrate an effective experimental protocol for the evaluation of the radiation induced degradation of the electronic performances of devices based on the IBIC technique and the relevant physical model, which is suitable to extract information on the effective radiation hardness of semiconductor materials.

10:30 - 11:00 --- Break ---

11:00 - 12:30 **Jyrki Raisanen** / *University of Helsinki, Finland*
Defect characterization by positron annihilation spectroscopy
The methods and principles of vacancy type point defect characterization by positron annihilation spectroscopy (PAS) are described. The basic processes related to fast positron thermalization in material are followed. Positron sources and the set requirements for them are discussed. The variations of PAS are introduced including positron life-time spectroscopy and techniques based on measurement of the 511 keV annihilation line energy spectrum. The discussed methods based on the momentum distribution include Doppler broadening and angular correlation of the annihilation quanta. The information that can be extracted by the various techniques is pointed out. Finally, the slow positron beam technique is introduced including positron moderation as well as the capabilities of this approach. The facility constructed at Helsinki University enabling point defect production by proton irradiation and in situ positron spectroscopy at low temperatures is described. Examples of studies conducted employing the facility and typical PAS studies published in the literature are shown.

12:30 - 14:00 --- Lunch Break ---

14:30 - 16:00 **Milko Jaksic** / *Rudjer Boskovic Institute, Zagreb - Croatia*
IBIC experiement, examples
In addition to many of ion beam analysis techniques that employ focused ion beams for the analysis of sample composition, microprobe technique IBIC (Ion Beam Induced Charge) provides information about the charge transport properties in the studied semiconductor samples. After charge carriers have been created along the trajectory of every single ion that is entering the sample and in the presence of internal or externally applied electric field, a charge signal is induced and measured at the sample electrodes. By knowing the exact position of every single ion and by using the measurement of the induced signal height and shape, imaging of charge transport properties of studied material can be performed. Many examples of IBIC applications in its frontal and lateral modes, application of technique to studies of different materials and devices, and in particular IBIC monitoring of radiation damage creation will be presented.

16:00 - 16:30 --- Break ---

16:30 - 17:30 **Poster presentation**

Thursday, 16 August 2012 (Room:Adriatico Guest House Kastler Lecture Hall)

- 09:00 - 10:30** **Gyorgy Vizkelethy** / *Sandia National Laboratory, Albuquerque - United States of America*
Radiation effects in microelectronic devices
Microelectronic devices and detectors are exposed to harsh radiation environments in space and in large accelerators. Radiation can cause several effects that will lead to the degradation and malfunction of these devices. This lecture will give an introduction to the effect of radiation on microelectronic devices including single event effects. The use of ion beams in the study of these radiation effects will be presented with examples.
- 10:30 - 11:00** --- Break ---
- 11:00 - 12:30** **Ivana Capan** / *Rudjer Boskovic Institute, Zagreb - Croatia*
Electrically active defects in semiconductors induced by radiation
In this talk, an overview of the current research on electrically active defects in semiconductors introduced by ion implantation, electron, neutron and Gamma-radiation will be presented. The fundamental differences between damage introduced by those sources, from point-like to cluster-related defects, will be shown. The application of capacitance transient techniques such as Deep Level Transient Spectroscopy (DLTS) and high resolution Laplace DLTS for studying the electrically active defects will be explained. The invention of DLTS, and later an improvement with Laplace DLTS which gives an order of magnitude better energy resolution has meant an enormous breakthrough in the study of electrically active radiation defects in semiconductors.
- 12:30 - 14:00** --- Lunch Break ---
- 14:00 - 15:30** **György Vizkelethy** / *Sandia National Laboratory, Albuquerque - United States of America*
Radiation damage in bipolar junction transistors
In this lecture the application of the previous lectures will be presented for a special case, radiation damage in bipolar junction transistors (BJTs). It will be shown how to use the previously presented methods (modeling ion solid interactions, various materials science methods, etc.) in a real life research project.
- 15:30 - 16:00** --- Break ---
- 16:00 - 17:00** **Poster presentation**

Friday, 17 August 2012 (Room:Adriatico Guest House Kastler Lecture Hall)

- 09:00 - 10:30** **Ivana Capan** / *Rudjer Boskovic Institute, Zagreb - Croatia*
Radiation induced defects in semiconductors: Optical study
Besides electronically active defects, radiation introduces defects which give rise to a level falling in the valence or conduction band, and therefore are not active. However, such radiation induced defects affect the optical properties of the semiconductor. Absorption spectroscopy may provide useful chemical and structural information, particularly when applied at cryogenic temperatures. One important advantage of photoluminescence (PL) spectroscopy is its high spectral resolution, which renders the technique sensitive to isotope or mechanical stress effects. In this talk, an overview of radiation induced (gamma rays, electrons, protons, ions) studied by IR and PL will be given.
- 10:30 - 11:00** --- Break ---
- 11:00 - 12:30** **Paolo Olivero** / *University of Turin, Italy*
Ion Beam Lithography I.
The basic concepts on the employment of keV and MeV ions for the micro- and nano-fabrication of advanced materials will be introduced, with comparisons with standard lithographic techniques. The current state of the art on most significant applications of ion beam lithography in materials of widespread use (such as silicon and photo-resists) will be reviewed.
- 12:30 - 14:00** --- Lunch Break ---

14:00 - 15:30 **Paolo Olivero / University of Turin, Italy**
Ion Beam Lithography II.
Following the previous introductory lecture, a case study will be discussed on the employment of focused ion beams for the microfabrication and functionalization of a specific innovative material, such as artificial diamond. The extreme physical properties that make diamond suitable for applications in advanced technological applications also pose significant limitations to its fabrication with conventional techniques, therefore ion beam lithography qualifies as an ideal tool to micro-structure and functionalize this material.

15:30 - 16:00 --- End of the 1st week tutorial ---

Monday, 20 August 2012 (Room:Adriatico Guest House Giambiagi Lecture Hall)
Chairperson: R. Smith

08:30 - 09:00 **Andrej Zeman / IAEA, Vienna - Austria**
Role of nuclear science and technology: IAEA CRPs, Technical Meetings and trainings

09:00 - 10:00 **Steve Zinkle / Oak Ridge National Laboratory, United States of America**
Fundamental aspects of radiation damage of nonmetallic materials
Ionizing and displacive irradiation produces a variety of effects at the atomic scale in nonmetals. During prolonged exposure, these atomic-scale effects can lead to pronounced property changes in materials. The average primary knock on atom energy of the atomic collision and exposure temperature can have a pronounced effect on the microstructural changes that occur during irradiation. In addition, the ionizing radiation component can modify the defect production, migration and resultant microstructural evolution. This presentation will review the fundamental aspects of defect production and microstructural evolution of inorganic materials, and will highlight commonalities and differences associated with ion beam and neutron irradiation of materials. A brief summary of radiation degradation mechanisms that can be induced by irradiation will also be given. Similarities and differences with radiation damage phenomena in metals will be summarized

10:00 - 10:30 --- Break ---

10:30 - 11:30 **Steve Zinkle / Oak Ridge National Laboratory, United States of America**
Nuclear technology applications of ceramics, composites and other nonmetallic materials
Inorganic nonmetallic materials are useful for a wide variety of nuclear technology technologies, ranging from nuclear fuels to functional applications. For example, mineral insulated cables (e.g., coaxial cables) are routinely used to carry electrical signals in high radiation and/or high temperature environments. Fiber optic cables and optical windows are also used in a variety of accelerator and reactor systems. Ceramics containing neutron-absorbing elements (e.g., ZrB₂ or B₄C) are useful for reactivity control in some reactor systems. Ceramics have several favorable attributes that make them promising candidates for advanced fuel systems such as inert matrix fuels and other microencapsulated fuel forms (e.g., TRISO particle fuels), and are proposed as a potential tritium breeding material for future deuterium-tritium fusion reactors. Ceramic composites such as carbon fiber reinforced graphite and SiC fiber reinforced SiC matrix composites offer a variety of attractive properties for structural applications in demanding high temperature, high radiation environments. An overview of the diverse applications of ceramics and composites in nuclear technology will be given.

11:30 - 12:30 **Vladimir Skuratov / Joint Institute for Nuclear Research, Dubna - Russian Federation**
Effects of heavy ion irradiation and simulation of fission fragments impact
Structural modifications induced by fission products, i.e. atoms with a mass ranging from 80 to 155 and an energy of about 100 MeV, still remain uncertain because the effects cannot be investigated using classical low-energy ion implanters. To date, only limited data concerning the microstructural response of insulators to ion irradiation of fission energy are available and external bombardment with energetic ions offers an unique opportunity to simulate fission fragment-induced damage. In this lecture, an overview of recent experimental results on radiation stability of nuclear ceramics and oxides against high energy ($E > 1$ MeV/amu) heavy ion irradiation will be presented.

12:30 - 14:00 --- Lunch Break ---

- 14:00 - 15:00** **Sheila Gonzalez** / *European Fusion Development Agreement (EFDA), Garching - Germany*
Overview of non-metallic materials for fusion applications (part I)
 In Fusion reactors a significant radiation field will be present. The ignited plasma will give rise to high energy neutron and gamma radiation fluxes, extending well beyond the first wall, together with an intense particle flux on the plasma facing materials. The radiation field will induce numerous different types of defects in the materials through displacement and ionization processes. In addition transmutation products from the nuclear reactions will build up with time representing impurity changes in the materials, as well as a source of possible activation. All these processes have very important consequences from the point of view of the machine operation, lifetime and reliability. Defect creation causes changes in the materials, and therefore in their properties. Radiation induced modification of the material properties is of course a technological problem, but is also an attractive phenomenon from the point of view of the basic physics and the understanding of the basic processes which occur in the materials subjected to a field of radiation. It is important to remember that the nature of non- metallic materials makes them highly sensitive to both ionization and displacement damage, with the result that the properties of interest may be severely modified even at low dose rates and for low doses, and that these materials are required in critical components of a number of different systems, such as high power RF windows (ICRH, ECRH), neutral beam injection (NBI) system, etc.. Hence changes in their properties may have serious consequences for the viability of the machine. Also ceramic breeders materials suffer severe degradation of their properties due to radiation.
- 15:00 - 16:00** **Vladimir Skuratov** / *Joint Institute for Nuclear Research, Dubna - Russian Federation*
SSwift heavy ion irradiation of nanostructured materials
 High energy heavy ion irradiation is a powerful tool for modification of semiconductor and metallic nanoparticles in oxide matrixes as well as oxide particles in metallic materials. In first part of this talk, swift heavy ion-induced changes in structure, electrical and optical properties of Si and Ge nanoclusters in SiO₂ layers are discussed. Second part of presentation is devoted to microstructural examination of nanostructured ceramics and oxide particles in oxide dispersion strengthened alloys irradiated in the electronic stopping regime.
- 16:00 - 16:30** --- Break ---
- 16:30 - 17:30** **Final presentation and evaluation of posters**

Tuesday, 21 August 2012 (Room:Adriatico Guest House Giambiagi Lecture Hall)
Chairperson: S.Zinkle

- 09:00 - 10:00** **Roger Smith** / *University of Technology, Loughborough - United Kingdom*
Principles of classical atomistic molecular dynamics computer simulations
 In this lecture I will describe the basic elements of the main techniques that are used to model ballistic collision phenomena in non-metallic condensed matter using classical molecular dynamics. Such simulations have been very successful at modelling the collisional processes and damage that can occur during the ballistic phase of a collision cascade. The history of the subject will be discussed along with the way in which molecular dynamics simulations have developed from the first simulations carried out by Vineyard's group at Brookhaven in the early 1960's. The main computer codes used in these simulations will be described along with details of the algorithms that are needed to implement the methods. The topics will include a brief overview of numerical integration algorithms for Hamiltonian systems, temperature control, optimisation methods, numerical tricks that can speed up the simulations and the latest potential functions that are used, including variable charge potentials.
- 10:00 - 10:30** --- Break ---
- 10:30 - 11:30** **Sheila Gonzalez** / *European Fusion Development Agreement (EFDA), Garching - Germany*
Overview of non-metallic materials for fusion applications (part II)
 Abstract ditto part I
- 11:30 - 12:30** **Thierry Wiss** / *European Commission, Joint Research Centre, Eggenstein-Leopoldshafen, Germany*
Overview of ITU programmatic activities related to the radiation damage of nuclear materials
 To be decided
- 12:30 - 14:00** --- Lunch Break ---

14:00 - 15:00

Wim Bras / *European Synchrotron Radiation Facility, Grenoble - France*

Synchrotron radiation interactions with soft condensed matter and ceramics

Synchrotron radiation is a high intensity radiation source which spatially, for the highest flux beamlines, is limited to beam sizes of at most several hundreds of microns. This can range over a large part of the electromagnetic spectrum from several hundreds of electronvolts to about 200 keV photons. A substantial number of synchrotron radiation laboratories offer access to a wide range of external users whom can perform experiments there which are not feasible with conventional X-ray radiation sources. In practice the majority of experiments that are carried out still utilize wavelengths not far removed from the X-ray energies, though not intensities, available from conventional X-ray sources, i.e. the photon energy range $5 < E < 25$ keV. Although X-ray in the energy range mentioned above are relatively benign, for the materials under study, compared to for instance electron microscopy, one cannot ignore the effects that are induced by these intense beams on the materials under investigation. These effects are especially noticeable with materials which are not purely crystalline and in which one can find a large amount of disorder or which are amorphous. However, even crystalline materials are not completely impervious to the effects of high intensity X-ray beams. Problems are not only encountered in the form of radiation damage to the samples but in some cases structure formation is even induced. There can also be substantial effects on the kinetics from time-resolved processes. Some of the interaction effects of high intensity synchrotron beams with a variety of materials will be discussed.

15:00 - 16:00

Sheila Gonzalez / *European Fusion Development Agreement (EFDA), Garching - Germany*

Combination of experimental tools and computer modelling for investigation of radiation damage - fusion applications

Using presently available scientific concepts, modelling tools based on existing and new mathematical algorithms and computer facilities have been developed over the last decades. To guarantee robustness, models must be grounded in physics and, as far as feasible, at the scales where the latter is most fully ascertained, this often being ? though not invariably so ? that of the atom, the more so since irradiation damage generation and evolution mechanisms are precisely induced at this scale. Ab-initio computation of electronic structures allows the basic properties (structure, formation, migration) of point defects to be arrived at. This has made possible the full modeling of self-diffusion, as of the crucial effects of impurities. Molecular dynamics is the basic tool for the investigation of ballistic damage processes, however its effectiveness is dependent on the quality of the interatomic potentials used. As regards insulators, moreover, the ab-initio approach, i.e. an approach based on rigorously taking into account the quantum character exhibited by physics at the atomic scale, is indispensable if electronic effects are to be taken on board, in particular the damage due to particles other than high-energy neutrons, electrons, and photons. Predictions of long-term microstructural evolution kinetics, rely on already highly developed models, that have shown good performance with respect to metals, application of which to ceramics, however, is only just beginning. The understanding, and modeling of mechanical behavior are likewise far more advanced for metals than for ceramics, however the multiscale approach, starting from the atomic scale, is still barely at an initial stage. At the same time, modeling must be closely coupled with experiment. Aside from gaining the relevant data as to behavior subsequent to neutron irradiation for the materials selected, it is indispensable to conduct a targeted experiment drive, aimed at ascertaining basic physical properties, and behaviors, and at the parametrization, and validation of the models. Thus, charged-particle irradiation ? involving ions, and electrons ? affords the possibility of mimicking, and analyzing, in detailed fashion, damage mechanisms in small, inactivated samples, which are thus amenable to a whole range of measurements, and observation, from the atomic scale up, both in situ, and ex situ.

16:00 - 16:30

--- Break ---

16:30 - 17:30

Wim Bras / *European Synchrotron Radiation Facility, Grenoble - France*

Synchrotron radiation based techniques for the study of structural radiation damage

There are many X-ray based experimental techniques that can be used to study material characteristics. For several of these experiments can be carried out in real time whilst the material is subjected to manipulations that mimic damage inducing processes. These processes can range from chemical (i.e. corrosion studies), via mechanical (i.e. deformation, stress/strain) to purely physical (i.e. radiation damage). It is rare that one is in the situation that radiation damage can be studied in real time. However, when care is taken one can prepare radiation damaged material in such a way that the radiation damage is frozen in until a trigger, like a thermal treatment, releases these defects and the evolution of the primary effect to larger scale structure, which will have an effect on the morphology and macroscopic mechanical stability, can be studied in real time. This can render information relevant to the functioning of mechanical components in high radiation and environmentally extreme, with respect to temperature and pressure, conditions. An oversight of some of the relevant experimental techniques will be given.

Wednesday, 22 August 2012 (Room:Adriatico Guest House Giambiagi Lecture Hall)

Chairperson: W.Bras

09:00 - 10:00

Steve Zinkle / Oak Ridge National Laboratory, United States of America

Effects of neutron and gamma irradiation on degradation of nonmetallic materials for high temperature applications

Numerous degradation mechanisms can occur in inorganic nonmetallic materials as a result of exposure to ionizing and displacive irradiation. These include prompt or low-dose changes in physical properties such as radiation-induced electrical conductivity and optical properties. Other radiation degradation phenomena include amorphization (and more generally, phase instabilities), decrease in thermal conductivity, volumetric swelling, decrease in strength and/or fracture toughness, irradiation creep, and high temperature helium embrittlement. This presentation will provide a summary of the diverse effects of neutron and gamma irradiation on the physical and mechanical properties of monolithic and composite inorganic solids. The fundamental physical processes responsible for the various degradation phenomena (e.g., electronic ionization of impurities or atomic displacement damage) will be summarized.

10:00 - 10:30

--- Break ---

10:30 - 11:30

Sheila Gonzalez / European Fusion Development Agreement (EFDA), Garching - Germany

R&D and qualification of non-metallic materials for DEMO reactor (long term operation conditions)

Non-metallic materials will be needed in radiation-hard components for diagnostic, H&CD, and other systems on DEMO and Power Plants. Up to now, there is enough information to allow one to make recommendations for insulator applications not only in ITER, but also to identify potential problem areas for future fusion devices. For thermo-mechanical properties (strength, swelling, thermal conductivity) data is available for doses > 1 dpa, however in general for the important physical properties which degrade at far lower doses, data is only available for doses $\ll 1$ dpa, corresponding to ITER expectations. In the case of ITER the maximum expected total dose for the numerous insulating components will be at most 0.3 dpa, and < 10 GGy (? 1/10th first wall dose), with the magnetic diagnostics suffering the highest radiation level. From the anticipated increases in the first wall total displacement damage for DEMO and Power Plant (< 3 dpa for ITER, ? 80 for DEMO, ? 150 for Power Plant), and assuming a Tokamak type device, this would lead to total doses for the most exposed insulators of about 8 dpa, 250 GGy (DEMO) and at least 15 dpa, 470 GGy (PP). From all the available data these elevated radiation doses would degrade even the mechanical properties (strength, swelling) of the most radiation resistant refractory oxides to very high levels, as well as introducing large concentrations of transmutation impurities.

11:30 - 12:30

Alessandro Fraleoni / ELETTRA, Trieste - Italy

Organic semiconducting single crystals: model organic semiconductors and novel X-rays detectors

Organic semiconducting single crystals (OSSCs) represent both promising building blocks for organic electronics-enabled devices and model systems for understanding charge transport in organic semiconductors. Nonetheless, OSSCs are surprisingly little studied with respect to their potential importance, and to more ?en vogue? organic semiconductors, although recent technological developments allowing to fabricate OSSCs-based devices by inkjet printing could catalyze a more general interest for the topic. Solution-grown OSSCs revealed recently interesting technological properties (such as three-dimensional anisotropic mobilities and ability to directly detect X-rays), and the possibility to get unprecedented insights into molecular mechanisms of charge transport via synchrotron-enabled infrared analysis. Therefore, some basic studies over OSSCs properties and features, and on their applications in the field of X-rays detection, with particular regard to their radiation hardness, will be reviewed. These topics will be discussed also in relation with the crystallographic structure of the considered OSSCs.

12:30 - 14:00

--- Lunch Break ---

14:00 - 17:30

ELETTRA : Technical tour

Thursday, 23 August 2012 (Room:Adriatico Guest House Giambiagi Lecture Hall)

Chairperson: T. Wiss

09:00 - 10:00

Thierry Wiss / *European Commission, Joint Research Centre, Eggenstein-Leopoldshafen, Germany*
JRC testing facilities and experimental tools for study of radiation damage

Most of the properties of nuclear fuels are modified during their reactor irradiation due to the numerous fissions and thermal gradient. The safe operation of nuclear fuels especially in abnormal conditions or to increased burnups to optimize their economics and environmental impact requires a thorough knowledge of their in-reactor aging. The formation of radiation damage is a complex process due to the nature of the different sources like fission fragments, alpha-decaying actinides or beta-decaying fission products. Single effect studies to tackle specifically radiation damage effects from these different sources are performed using ion-implantations but also doping with radioactive elements. The effect of radiation damage on the thermal-conductivity degradation of nuclear fuel could be demonstrated using UO₂ samples doped with ²³⁸Pu. The microstructure evolution of the nuclear fuel towards the high burnup structure could be partly explain by ion-implantation studies. Aging of waste conditioning matrices like zirconolite or pyrochlore has been accelerated by doping these ceramics with ²⁴⁴Cm or ²³⁸Pu. Characterization tools like Transmission or Scanning Electron Microscopy, X-ray diffraction, thermal diffusivity or heat capacity measurement have been used on irradiated fuel samples as well as on doped or ion irradiated samples to study the elastic or inelastic energy losses and their effect in various type of ceramics.

10:00 - 10:30

--- Break ---

10:30 - 11:30

Roger Smith / *University of Technology, Loughborough - United Kingdom*
Introduction to atomistic multi-scale modelling

In this lecture, ways in which the atomistic simulations can be extended both in space and in time will be described. For extensions in space, parallelisation methods will be described as well as how it is possible to link MD to finite element methods. However, the bulk of the lecture will be to describe the latest long time scale techniques by which the time scales of radiation effects can be extended from those accessible by classical MD. In MD the largest time step that can be used in a numerical integration scheme is of the order of 10-15s. Thus to simulate even 1s of real time would require 10¹⁵ integration steps which is computationally infeasible. To overcome this problem it is necessary to calculate the transition energy barriers between local minima on n-dimensional potential energy surfaces and the frequency of occurrence of such events. A review of the methods that can do this will be described. This will include methods that do not rely on a prior knowledge of what the transition may be. Such barriers can be used to determine diffusion coefficients required for rate theory models and implemented into on-the-fly kinetic Monte Carlo techniques.

11:30 - 12:30

Vladimir Skuratov / *Joint Institute for Nuclear Research, Dubna - Russian Federation*
Structural effects of dense ionization: theoretical model/ experimental verification/ applications

Experimental data concerned the most prominent effect of dense ionization in non-metallic solids - latent tracks formation, are usually interpreted in framework of thermal-spike models. In this talk we discuss different thermal-spike models and their application for evaluation of latent track parameters and electronic excitation effects in insulators. Some examples of industrial applications of swift heavy ion beams will be presented.

12:30 - 14:00

--- Lunch Break ---

14:00 - 15:00

Thierry Wiss / *European Commission, Joint Research Centre, Eggenstein-Leopoldshafen, Germany*
Current R&D activities on ceramic fuel

In order to assess safety and performance of fuels for current or future types of nuclear power reactors it is essential to be able to measure relevant fuel properties such as thermal transport, fission gas behaviour, and mechanical properties and to correlate their evolution with microstructural changes as a function of burnup and irradiation conditions. An overview on the characterization methods used or under development in ITU and on the main results from studies focused on nuclear fuels is presented. In the perspective of future developments of advanced reactors and related fuel cycles, as envisaged by international efforts like e.g. GenIV, the focus of this type of studies is now shifting from standard, low/medium burnup LWR UO₂ fuel to cover high/very high burnup, Pu-containing fuels, starting with MOX, and including non-oxide systems like e.g. nitrides, carbides but also minor actinide-containing fuels are also considered. A strong effort is ongoing to adapt or upgrade experimental facilities and methods optimized to the study of UO₂-based pellets to the new concepts. An overview of developing activities in this area is also provided.

- 15:00 - 16:00** **Roger Smith** / *University of Technology, Loughborough - United Kingdom*
Application of molecular dynamics and long time scale atomistic methods to radiation simulations in non-metallic condensed matter
The methods described in Lectures 1 and 2 will be applied to the study of radiation damage in MgO, Er₂O₃ and magnesium aluminate spinel, initiated by keV energy knock-on atoms. The structure of the collision cascades in these materials will be described along with some non-intuitive results concerning the diffusion of defect clusters and how the diffusion mechanisms can be further used in rate theory models. In addition variable charge potentials will be implemented to show how oxide coatings (TiO₂ and ZnO) behave when subjected to bombardment by energetic atoms, especially how the growth processes in a magnetron device occur over realistic time scales and how it is possible to use the simulation techniques to inform experimentalists of the conditions required for optimal crystalline growth.
- 16:00 - 16:30** --- Break ---
- 16:30 - 17:30** **Vladimir Skuratov** / *Joint Institute for Nuclear Research, Dubna - Russian Federation*
Real-time characterization and high energy ion irradiation testing of non-metallic materials
Accelerator based real-time methods play important role in characterization of dynamic processes during irradiation. In this lecture we discuss the results of real-time experiments aimed at studies of radiation damages and mechanical stresses in non-metallic materials induced by swift heavy ions (LiF, Al₂O₃, polymers).

Friday, 24 August 2012 (Room:Adriatico Guest House Giambiagi Lecture Hall)
Chairperson: A.Zeman

- 09:00 - 10:00** **Steve Zinkle** / *Oak Ridge National Laboratory, United States of America*
Ongoing challenges in development of advanced nonmetallic materials for nuclear applications
This presentation will summarize some of the key fundamental obstacles to application of advanced nonmetallic materials in nuclear applications. These barriers are based on two general issues: low ductility and toughness of ceramics (which generally limits their applicability to nonstructural applications), and radiation-induced degradation of properties (e.g., electrical conductivity, optical transmission, fracturing due to anisotropic swelling, etc.). A variety of approaches are being utilized to mitigate these barriers and to enable broader use of nonmetallic materials in nuclear applications. For example, ceramic composites provide adequate engineered toughness for many structural applications, although robust engineering design rules for structural operation involving public safety still need to be developed. Appropriate selection of radiation-resistant materials (e.g., doped oxides for optical applications, or isotropic structures rather than hexagonal close packed structures for structural applications) is being pursued to enable broader use of nonmetallic materials for nuclear applications.
- 10:00 - 10:30** --- Break ---
- 10:30 - 11:30** **Presentations of selected papers - winners of poster sessions, questions and answers**
- 11:30 - 12:30** **Closing ceremony: Award of certificates**
- 12:30 - 14:00** --- Lunch Break ---