Modelling of Radiation-Induced Effects in Nuclear Materials

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This research project is based on the modelling of radiation-induced effects in nuclear materials based on the use of energetic ion beams and computational tools. In fact, ion beams are versatile tools, and they can address the following major issues: (i) irradiation-induced damage on the various regimes of slowing-down of bombarding ions (electronic and nuclear energy loss); (ii) incorporation of selected impurities by ion implantation; (iii) investigation of the structural and microstructural evolution of solid using nuclear microanalysis techniques (Ion Beam Analysis). Let us stress that the choice of the beam nature and energy allows us to reproduce pure irradiation conditions, as well as pure doping ones, but also to reproduce a wide range of situations where both the physical and chemical processes are mixed. The main idea is to reproduce the physical and chemical features of a solid exposed to given irradiation conditions. Different classes of nuclear materials are of special interest in collaboration:

i. uranium dioxide (UO_2), the nuclear fuel, since we already collected a lot of experimental data on this system whose strong radiation tolerance still needs to be elucidated concerning mechanisms of the structural reorganisation at the atomic scale (for instance, the formation of the High Burnup Structure in UO_2 nuclear fuel still deserves detailed investigations as well as the role played by chromium in accident tolerant fuels). In particular, the favourable lattice location of Cr into UO_2 is currently being investigated. Chromium is incorporated into the solid by ion implantation at the IJCLab MOSAIC facility and its location in the UO_2 crystalline structure is revealed using ion channelling experiments by measuring PIXE (Particle Induced X-ray Emission) to detect Cr as well as RBS (Rutherford Backscattering Spectrometry) to collect U and O signals, mainly to determine defect profiles. Basically, while investigating to main crystallographic directions for both matrix (U and O) and added element (Cr), the location of Cr can be obtained using a triangulation method. First tests were performed: angular scans were recorded across the main crystallographic axis and major planes and the Cr signal was clearly identified. Analysis of the data is currently under progress using the McChasy-1 software and it will be developed in 2024.

ii. nickel (and Ni-based superalloys) as a key material for the vessel and internal parts of the nuclear reactor (fuel subassemblies and structures). The proposed strategy to achieve a description as complete as possible of the behaviour of a solid exposed to irradiation requires the use of a very simplified model system (here we select intentionally monocrystalline solids) irradiated in well-defined conditions provided by energetic ion beams delivered by accelerators and submitted to the most advanced characterization techniques (ion channelling and transmission electron microscopy – both techniques can be performed in-situ or ex-situ at the MOSAIC facility) to identify the radiation defects and to follow their evolution. One of the key points is the capability to model extended defects (e.g., dislocation loops and lines) realistically by creating virtual crystals defined through MD simulations and by comparing them with experimental data. Such an approach requires a new Monte Carlo simulation code (McChasy-2), which is capable of working with large (nm-size) structures. The development of such code will be the milestone of the project.

In this regard in the second generation of the McChasy program, the possibility to create large virtual structures by merging and propagating, according to the user-specified distribution, the MD cells containing dislocation loops oriented along the (111) plane in Ni and Ni-based alloys was successfully implemented.

iii. Apatite is a class of solids considered for nuclear waste immobilization. Indeed, the crystalline structure of apatite allows the substitution of matrix cations with fission products and actinides. We have investigated the radiation stability of fluorapatite single crystals under alpha decay at the MOSAIC facility using Bi and He ions, to simulate the heavy recoil nucleus and the alpha particle. Radiation damage was quantitatively characterized using channelling experiments and MC simulations using the McChasy code. The nature of the disorder was monitored using TEM. The development of the possibility of adding bubbles of noble gases (in different phases) on the way of channelling ions in both the first and second generations of the simulation codes is in the testing phase. An in-depth modelling of the radiation-induced damage at any step in the evolution of the apatite solid is in progress and it will be completed in 2024.

iv. Steels and alloys used in nuclear installations. An obvious question related to their use in nuclear engineering is their radiation resistance and modification of functional properties, mainly mechanical, by accumulation of the radiation defects. These properties were studied essentially by nanoindentation technique, in the lesser extent by Transmission Electron Microscopy. These studies will gain a more marked impetus in the 2024 due to significant investments in the NCBJ: new TEM allowing for in-situ analyses at high temperatures (up to 1000 °C) and possibility to perform in-situ tensile tests in TEM column and new tensometric stage permitting the irradiation of the samples under stress. This stage allows one to apply tensile or compressive stress up to 5N to the samples and can be used in vaccum (e.g. irradiation chamber of ion accelerator) or as an element coupled with XRD or Raman devices. It will allow thus to analyse the role of stress on kind and amount of radiation defects created by irradiation.