HORIZON 2020

MULTISCALE MODELLING FOR FUSION AND FISSION MATERIALS

Reporting

Project Information

M4F

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Project website

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Project closed

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CENTRO DE INVESTIGACIONES ENERGETICAS MEDIOAMBIENTALES Y TECNOLOGICAS
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Periodic Reporting for period 3 - M4F (MULTISCALE MODELLING FOR FUSION AND FISSION MATERIALS)

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Summary of the context and overall objectives of the project

The sustainability of nuclear fission energy will be ensured when Generation IV (GenIV) systems are deployed. Thermo-nuclear fusion represents in the longer term a virtually inexhaustible source of

energy, with potentially very high standards of sustainability, efficiency and safety. Despite differences between GenIV fission and fusion reactors, in both technologies materials will be exposed to high levels of irradiation and high temperatures, in contact with potentially aggressive non-aqueous coolants. Thus, several materials issues are common.
In this context, the M4F project (Multiscale modelling for fusion and fission materials) promotes cross-fertilization between the nuclear fission and fusion materials modelling and characterization communities, to work on structural materials that are of interest for both, namely ferritic/martensitic (F/M) steels. These offer excellent radiation-induced swelling resistance and thermal properties, as compared to austenitic steels, but suffer from low temperature neutron irradiation hardening, embrittlement and loss of uniform elongation, with impact on design rules and codification activities.
Specifically, two are the overarching objectives of the M4F project:
O-a) Develop physical understanding and predictive models of the origin of localised deformation under irradiation in F/M steels and its consequences on the mechanical behaviour of components, starting from modelling and understanding the changes caused by irradiation on the microstructure and microchemistry of the materials involved;
O-b) Develop a methodology to use ion irradiation as a tool to evaluate radiation effects on materials, minimising artefacts with respect to neutron irradiation experiments and allowing evaluation of not only microstructural change, but also mechanical property changes, via nanoindentation, applying it to F/M steels.
The complexity of the processes that drive the production and evolution of microstructural damage induced by neutron irradiation and the consequences it has on the material's behaviour require large R&D efforts, that advise synergies to be exploited and collaboration to be promoted between fusion and fission materials research groups, applying a multidisciplinary approach. In it, both modelling and experiments at different scales are integrated to enable the understanding of the complex phenomena associated with irradiation damage in F/M steels, providing input to design codes.

Work performed from the beginning of the project to the end of the period covered by the report and main results achieved so far

During this first period the main objective was to launch properly all activities, including when required recruitment of PhD students and post-docs. In particular, the ion implantation experiments have been planned and designed: materials selection and procurement, sample preparation, ion type and energy, irradiation conditions, and so on. The irradiation experiments will be performed and completed before end 2019. From the modelling point of view, effort has been devoted to:
- use advanced simulation tools for the assessment of differences and similarities between ion (including proton) and neutron irradiation conditions, in terms of type of primary damage created, concluding that the conditions that have been chosen for the ion irradiation experiments within the project (ion energy) are very suitable to mimic neutrons;
- develop advanced interatomic potentials for the study of e.g. the interaction of dislocations with large lattice defects such as prismatic loops decorated by C in Fe-Cr alloys or the interaction of dislocations with grain boundaries;
- simulate by molecular dynamics models of nanoindentation processes at finite temperatures, introducing explicitly radiation defects;

- further advance in microstructure evolution models to enable the simulation of chemically complex systems in volumes comparable with those affected by implanted ions.
Tasks like these will provide the atomistic input for larger scale plasticity models, typically based in dislocation dynamics. Regarding these methods
- a new coupling between a DD code and a fast-Fourier transform (FFT) solver has been released and applied successfully to the simulation of dislocation microstructure case studies.
In terms of continuum finite element-based models:
- a new polycrystalline homogenization scheme, based on the experimentally observed channel structures for irradiated F-M steels, has been proposed;
- average tensile responses have been computed by means of full-field homogenization of polycrystalline aggregates with various numbers of grains, under soft and hard boundary conditions and for different strain rates;
- a suitable finite strain model enabling the description of large inelastic deformation has been identified and adapted to irradiated F/M steels;
- finite element models of deformation in nanoindentation have been set up, using a material model based on tensile test data, and the outcome compared with experimental observations of nanoindentation stress-strain responses.

Progress beyond the state of the art and expected potential impact (including the socio-economic impact and the wider societal implications of the project so far)

It is too soon to assess the progress that has been actually achieved beyond the state of the art. However, it is clear that the project is targeting very ambitious goals in terms of modelling, in two senses:
- the modelling tools that are used correspond to the latest advances in the field of multiscale modelling of, specifically, radiation-effects;
- the modelling and experimental activities are designed in a consistent way (experiments are amenable to modelling and models will be validated on them) and targeted to address a well-defined type of issue, namely plastic flow localisation and use of ions as surrogate for neutrons, including assessment of mechanical properties.
Ultimately, the success of the project will have to be measured in terms of support that the models and experimental procedures (mainly nanoindentation) provide, on the one hand, to the definition of design rules and thus codification for F/M steels and, on the other, the design of ion irradiation experiments, enabling also the assessment of the mechanical properties of the ion irradiated materials.
The former result will facilitate the use of F/M steels in the design of GenIV fission and fusion nuclear reactors; the latter will provide the bases to effectively screen materials with superior radiation resistance, thus opening the way to further improvements of materials performance, towards enhanced safety and efficiency of future fission and fusion systems.

Project Logo

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