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Nuclear Materials

SUB-PROGRAMME 4

Physical modelling and modelling-oriented experiments on structural materials

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Summary Research activity

SP4 is a cross-cutting sub-programme with SP1, SP2 and SP3. Its overall objective is to provide knowledge, data and tools needed to interpret correctly and extrapolate to real conditions the experimental results devoted to the qualification of materials subjected to reactor-like conditions selected in SP1, as well as to assist in the elaboration of fabrication routes for innovative materials performed in SP2 and SP3. The focus is on the understanding of the physical mechanisms that determine the response of the material under given conditions owing to the development of physics-based models and the deployment of modelling-oriented experiments. Physical phenomena related to the synergistic effect of irradiation, temperature and environment cannot be supposed to be linear. Incubation times or doses and thermally activated processes may determine the appearance of totally unexpected materials responses above a certain dose or temperature of when subjected to a combination of stresses of different type. Thus, a physics-based prediction of the behaviour of materials in the envisaged in-service conditions must be based on some degree of fundamental understanding of the basic mechanisms acting from the atomic to the macroscopic level and determining their response to the applied environmental, thermal and mechanical loads, while being exposed to neutron irradiation. The build-up of this knowledge is crucial for the safe operation and design of all future nuclear installations.

The ultimate goal of the subprogramme is to set firmer grounds in the development of models and correlations allowing safe extrapolation of experimental data from laboratory to operating conditions, beyond purely empirical approaches of unassessable reliability. The physics-based models considered in this subprogramme span all scales, from electronic structure calculations that make use of quantum mechanical approaches and physical-mathematical solving methods, to continuum models that use finite element solving methods. Modelling-oriented experiments using several advanced materials characterisation techniques are included. By looking carefully at the microstructural features and changes at different scales, examining materials after exposure beyond what is strictly needed for qualification, they aimed at providing information of physical mechanisms and correlation between changes at different scales. For a better understanding of mechanisms, the examination of model materials and the use of target experimental campaigns aiming at discriminating between acting mechanisms are very helpful.

The current research in this SP is defined by the on-going FP7/MatISSE project on F/M steels and 7 pilot projects (PP). Three PP are "pure" SP4 projects, namely:

- IOANIS (Ion irradiation as a neutron irradiation surrogate – Potential, challenges and limits)
- ICAR (The influence of initial microstructure/carbon distribution on the swelling and hardening of irradiated FeCrxC alloys)
- MARACAS (Simulation of Model Alloys Representative of AustenitiC stAinless Steel)

Four SP4 PP, on the other hand, were linked to one or two other sub-programmes, namely:

- SLIPLOC (multiscale modelling of slip localisation under irradiation), transversal to SP1;
- MOLECOS (modelling of heavy-liquid metal corrosion of steels), transversal to SP1;
- MOSEL (modelling steel embrittlement by heavy liquid metals), transversal to SP1;
- NINA (development and application of nano-indentation), transversal to SP1 and SP2 as well; This PP is described in SP2 DoW.

MatISSE, IOANIS and ICAR focus on ferritic/martensitic (F/M) steels, MARACAS on austenitic steels. SLIPLOC, MOLECOS, MOSEL deal with both steels. NINA, which is presented in SP2 DoW, focuses on F/M steels and ODS F/M steels.

List of abbreviations

AKMC	atomistic kinetic Monte Carlo
APT	atom probe tomography
CTEM	Conventional Transmission electron microscopy
DD	dislocation dynamic
DFT	density functional theory
DOMO	design-oriented modelling
EBSD	Electron backscattered diffraction
EDS	Energy dispersive spectroscopy
FIB-SEM	focussed ion beam scanning electron microscope
FTIR	fourier transform infrared spectroscopy
GB	grain boundary
GD-OES	glow-discharge optical emission spectroscopy
(G)SAS	(grazing-incidence) small-angle scattering (neutrons or X-rays)
HLM	heavy liquid metals
HLME	heavy liquid metal embrittlement
HRTEM	High resolution transmission microscopy
HVEM	High voltage electron microscope
ICP-MS	inductively coupled plasma mass spectrometry
IF	internal friction
KMC	kinetic Monte Carlo
LBE	lead bismuth eutectic
MD	molecular dynamics
MEGAPIE	megawatt pilot experiment
NI	nano indentation
ODS	oxide-dispersion strengthening/strengthened
OKMC	object kinetic Monte Carlo
PAS	positron annihilation spectroscopy
PBMO	physics-based modelling
PIE	post-irradiation examination
PP	Pilot project
RECD	rate equation cluster dynamics
SANS	small angle neutron scattering
SCMF	self-consistent mean field
SEM	scanning electron microscopy
SIMS	secondary ion mass spectroscopy
SRA	Strategic Research Agenda
TDS	thermal desorption spectroscopy
TEM	transmission electron microscopy
WDX	wavelength dispersive X ray spectroscopy
XRD	X rays diffraction

I. Background and objectives

Experiments on materials under conditions of relevance for fast reactors, such as those foreseen in SP1, SP2 and SP3, can be long, expensive and subjected to severe and strict safety constraints, especially when neutron irradiation is involved. Materials cannot in any case be subjected to all possible conditions potentially encountered when in service, particularly if synergetic effects need to be considered. Therefore, it is desirable that the experimental matrices for the qualification of materials should be based on a physical and mechanistic understanding, in order to optimise both the time and the financial frames, as well as the relevance of the experimental results obtained. Moreover, extrapolations from the experimental results with purely empirical correlations have a high risk of being unreliable. Extrapolations become acceptable, however, and overall the correlations used become more reliable, if guided by a background of understanding of the physical mechanisms that drive the response of materials at the different scales to the conditions they are subjected to. Such background of physical and mechanistic understanding also provides guidance to identify the most critical conditions under which materials should be tested, as well as to help in the identification of mitigation strategies. Finally, by understanding the processes that occur during the fabrication of materials, the manufacturing steps can be optimised and the properties of the final product improved, or new routes to fabrication can be devised.

Achieving this capability, however, requires a continuous effort in the direction of examining materials after exposure beyond what is strictly needed for qualification, by looking carefully at the microstructural features and changes, using a combination of advanced techniques, given that no single technique will give a complete picture of the situation because of the different length scales concerned. For a better understanding of mechanisms, moreover, the examination of model materials and the design of experiments aimed at discriminating between acting mechanisms is very helpful: these are the so-called modelling-oriented experiments. Specifically for the study of irradiation effects, ion irradiation is a very suitable tool in this framework. As an important complement, computer simulation tools, based on physical modelling schemes ranging over different scales are nowadays available that allow complex physical processes to be modelled in great detail, providing a basis for the quantitative interpretation of the experimental observations, going in some cases also beyond what experiments can see. The physics-based models considered in this subprogramme span all scales, from electronic structure calculations that make use of quantum mechanical approaches and physical-mathematical solving methods, to continuum models that use finite element solving methods. This multiscale modelling approach reduces the number of parameters that need to be fitted, asymptotically aiming at eliminating the need to fit to experiments, although getting closer to this goal requires the elaboration of ever more refined models and simulation tools, the development of which is in the end justified by a cost-benefit analysis.

The development of models describing the behaviour of materials under irradiation, and under extreme conditions in general, has been and still is an important part of a number of Euratom projects (e.g. FP6/PERFECT, FP7/GETMAT, FP7/PERFORM60, FP7/ MatISSE, …), including fusion research (IREMEV). The importance of modelling activities in connection with innovative nuclear systems is also expressed in the SRA of the SNETP and is reflected in both the roadmap of NUGENIA [1] and of fusion energy [2]. Links with the industry exist at the level of Euratom projects related to materials for existing reactors (e.g. FP6/PERFECT and FP7/PERFORM60, which were coordinated by a utility, EDF). The introduction of these activities among the backbones of the JPNM of EERA allows a connection to be established between fundamental research (academia) and industrial initiatives related to future nuclear systems.

The overall objective of this SP is thus to develop physical models and corresponding computational tools in support of the fundamental understanding of the processes that drive the behaviour of materials when subjected to the extreme conditions expected in fast reactors, as well as the processes of relevance for materials fabrication and treatment, in synergy with advanced microstructural characterization and by performing modelling-oriented experiments.

The models should eventually serve several purposes:

- Optimisation of experimental matrices for materials screening, characterisation and qualification.
- Elaboration of mechanistic correlations in support of design rules and materials codification.
- Identification of mitigation strategies.
- Optimisation of materials fabrication routes.

This SP is expected to be transversal to the previous three on structural materials. In several cases it may be disputable where the frontier is between this SP and the others. Broadly, it is considered that large scale semi-empirical modelling belongs more to other SPs, this one being focused on smaller scale physical modelling, but in fact the difference is often blurred. Because of this, often joint initiatives are taken between SP4 and other SPs on structural materials.

The past activities of this SP have been largely connected to the WP4 of the FP7/GETMAT project (ended in October 2013) and also, partially, with the FP7/PERFORM60 project (ended in September 2013). Most effort was devoted to the development of **physical models to simulate the microstructural evolution under irradiation in ferritic alloys**, containing an increasing number of substitutional alloying elements: mainly Cr, but also Cu, Mn, Ni, Si, and P, as well as C as interstitial alloying element. This entailed not only a detailed study of the atomic-level processes driving creation and evolution of radiation defects in complex alloys, but also an intense experimental activity on Fe-Cr-C model alloys, involving irradiation and subsequent post-irradiation examination. The main goal of these models was to establish a **physical correlation between microstructural evolution and radiation hardening**, as a cause of embrittlement. This focus is related with the proposed used of F/M steels in GenIV and fusion reactors, that suffer from radiation hardening. More broadly, however, the development of microstructure evolution models allows also other problems to be addressed, such as swelling, and to understand in a quantitative way processes such as radiation-induced segregation, radiation-enhanced/induced precipitation, and so on. The corresponding deliverables of, mainly, GETMAT, allowed the milestones for the 2011-2015 phase to be reached.

The **current research** in this SP is defined by the on-going FP7/MatISSE project on F/M steels and the PPs proposed in 2015. Three PP proposed in 2015 are "pure" SP4 projects, namely:

- IOANIS (Ion irradiation as a neutron irradiation surrogate – Potential, challenges and limits)
- ICAR (The influence of initial microstructure/carbon distribution on the swelling and hardening of irradiated FeCrxC alloys)
- MARACAS (Simulation of Model Alloys Representative of AusteniticC stAinless Steel)

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Now the **research is extended to austenitic alloys** and **addresses explicitly issues such as swelling and compatibility with HLM**, making an effort to move to larger scales. Indeed, only very recently did F/M steels disappear from the priorities for the ESNII systems. Therefore most attention was devoted to F/M alloys. Now the situation is changing. The structural materials of choice common to the first cores of all ESNII concepts in their current design are austenitic steels, 316L(N) for most components, and 15-15Ti (in several slightly different versions) for the cladding. Structural materials will receive low irradiation dose in ASTRID but at high temperature with helium production in some case. Even though the irradiation fluences are low, it is of prime importance for the 60-year design life demonstration to be able to predict the microstructure evolution that will alter its mechanical properties, in particular its creep and fatigue resistance on the very long term. Cladding will receive very high irradiation fluences, so void swelling may appear and limit the lifetime of this component. Swelling resistance is the main reason for the choice of 15-15Ti steels instead of 316 steels. Nevertheless, even with AIM1 alloys, swelling is such that at around 100 dpa the fuel will have to be removed from the reactor, whereas the burn-up is not complete. Extending the incubation regime is thus a key issue to increase the lifetime of cladding. In MYRRHA and ALFRED, corrosion represents a critical challenge in the use of heavy liquid metals (HLM) as coolants. Corrosion, dissolution and erosion by Lead and Lead-Bismuth that might have also implications of embrittlement are key issues to be addressed.

It is therefore important to understand on physical basis the evolution of the austenitic steel under irradiation, the influence of the microstructural evolution on their creep resistance on very long term and their compatibility with lead-bismuth eutectic in MYRRHA and lead in ALFRED especially at high temperature (>400°C).

Given the difficulty of getting data, the long time required for 60 yrs lifetime, the complexity to perform experiments on swelling resistance and on compatibility with HLM, but also to have access to the basic mechanisms, physical models for the microstructural evolution and its effect on the material properties combined with modelling-oriented experiments and advanced microstructural characterization techniques, are crucial to achieve predictive capability and to contribute to the elaboration of mitigating solution. Modelling of austenitic steels is much less mature than modelling of ferritic-martensitic steels mainly because conventional multi-scale approaches based on DFT calculations performed at 0K are difficult to follow for this system. A big effort is needed for these steels. The role and the influence of major elements and impurities on the behaviour of the steels together with synergies are essential to understand. At each scale, careful validation of the modelling has to be carried out owing to advanced characterisation. **MARACAS**, **SLIPLOC** and **MOLECOS** address these issues.

Moreover, wider use of microstructural examination is made, including an **effort to make ion irradiation an ever better performing tool to study radiation effects**: by combining models and experiments, the goal is to identify and understand the limits of ion irradiation as a neutron irradiation surrogate and developing strategies to obtain the most suitable conditions to be as close as possible to the microstructure that neutrons would produce.

Indeed, future nuclear applications like GEN IV fission reactors pose new materials challenges. The development and qualification of new structural materials for these applications require a profound understanding of the degradation mechanisms occurring in harsh environment of GEN IV reactors (fast neutrons, high doses, corrosive environment) and screening of a considerable number of materials to identify the most promising candidates. Both rely on comprehensive experiments with prototypic conditions and coupling with modelling to rationalize our understanding on physical basis. Ferritic/martensitic steels will be used for the hexagonal cans in ASTRID and are a long term option for cladding tubes when reinforced by oxides (ODS) or by fine MX particles because of their excellent swelling resistance and good thermal properties. Nevertheless, some key issues remain: low

temperature embrittlement, need to increase creep resistance, mitigation of the susceptibility to liquid metal embrittlement. The **WP2 of FP7/MatISSE** project focusses on the two first issues, namely, low temperature embrittlement and creep.
The limited availability of suitable neutron irradiation facilities as well as costs and time expenditure of neutron irradiation experiments give rise to an interest in alternative irradiation sources which allow experiments involving a wide range of irradiation conditions. The potential of ion irradiation to efficiently approximate neutron damage in structural materials and to serve as a tool for basic investigations and materials screening has long been recognized. However, by using a surrogate for neutron irradiation transferability issues are introduced both in terms of microstructure and mechanical properties. These transferability issues arise from factors such as damage rates which differ in several orders of magnitude, cascade morphologies but also carbon pollution or the limited penetration depth of the ions, which is in the range of a few micrometres, and the non-homogeneous displacement profiles...

To explore how PIE results for ion-irradiated materials can be transferred to neutron irradiation, identifying the limits of ions as a neutron irradiation surrogate and developing strategies to obtain equivalent experimental information for ion-irradiated and neutron-irradiated material are of primary importance. Coupling of targeted and systematic irradiation experiments on model alloys and steels with advanced characterization of the microstructure and modelling of the microstructural evolution will be exploited in order to identify the mechanisms responsible for the differences observed under ion and neutron irradiations. Also, in order to deduce information on mechanical properties from ion irradiation experiments, nanoindentation is specifically studied. The initial microstructure (ferritic or ferritc/martensitic) is also an issue. Depending on the initial microstructure (and the nominal C content), the defect formed after irradiation and their overall contribution to the degradation of the mechanical properties in 9%Cr steels and alloys may strongly differ. Targeted experiments of HLM embrittlement of steels in synergy with development of models are essential for providing physical understanding that will contribute to screening of new materials. **IOANIS**, **ICAR**, **NINA** and **MOSEL** address these different issues.

The SP has therefore a strong connection with SP1 in terms of materials and issues. At the moment the link with SP2 and SP3 is largely missing. A research agenda concerning modelling in support of ODS steels fabrication has been drafted some time ago, but has not led to any practical implementation. However, some activities on thermodynamic modelling in support of the development of CSE steels are proposed in the PP CREMAR. Very few modelling activities exist at the moment devoted to ceramics and those that exist are included in the JOISIC PP, in SP3.

[1] http://nugenia.org/docs/NUGENIA_roadmap.pdf
[2] http://www.efda.org/wpcms/wp-content/uploads/2013/01/JG12.356-web.pdf

II. Description of forseen activities

1. FP7/MatISSE project – High-Cr ferritic/martensitic steels

Ferritic/martensitic (F/M) steels will be used for the hexagonal cans in ASTRID and are a long term option for cladding tubes when reinforced by oxides (ODS) or by fine MX particles because of their excellent swelling resistance and good thermal properties. Nevertheless, some key issues remain as low temperature embrittlement and irradiation creep. These issues are addressed in the WP2 of FP7/MatISSE through two ongoing SP4 pilot projects (PP):

- MEFISTO deals with embrittling microstructural features that involve also microchemical processes, due to the effect of elements such as Cr, Ni, Si and P,[1] in order to make a correlation with radiation-induced hardening.

1 These elements were identified as important as a result of the WP4 of FP7/GETMAT.

- MOIRA addresses for the first time the effect of stress in microstructure evolution under irradiation using atomistic modelling, providing the tools and the knowledge to derive macroscopic models that predict irradiation creep strain.

The main objective of MEFISTO is to build knowledge on the effect of the composition on the type of phases that form under irradiation in high-Cr F/M alloys, their kinetics of formation, their effect on radiation-hardening (generally correlated with embrittlement), as a basis for mechanistic embrittlement correlations, similar to those developed for reactor pressure vessel steels used in LWRs. The work proposed is the logical extension and continuation of the work performed in GETMAT, where the focus was on FeCr alloys and, particularly, on the formation of Cr-decorated loops as hardening features.
More specifically, the work will address two issues:

- Study of the mechanism of formation of Cr-rich-NiSiP clusters, including a detailed description of the mechanisms of diffusion of the constituent chemical elements in Fe alloys, their possible role as precursors for complex phase formation, and their impact on radiation-induced hardening, using atomic and dislocation-level simulation tools.
- Design and performance of modelling oriented experiments on model alloys and, possibly, steels, in order to obtain detailed information on these clusters and their effect on radiation-induced hardening, thereby allowing the improvement and validation of the models, as well as setting the basis for the derivation of mechanistic embrittlement correlations.

These two issues are intimately correlated, as experiments provide information to develop models and models are used to rationalise experimental results.

The main objective of MOIRA is to develop and then apply atomic- and dislocation-level simulation tools to evaluate the relative importance of irradiation creep mechanisms, such as: stress-induced preferential absorption (SIPA) or nucleation (SIPN), anisotropic diffusion, dislocation climb&glide (deriving relevant dislocation mobility laws), slip bands. This will be done by:

- Studying atomistically the absorption of defects at dislocation loops and lines under given stress fields and the influence of the latter on stability and mobility of radiation defects.
- Using continuum viscoplasticity modelling coupled to lower scale models to determine the effect on (visco)plasticity of dislocation climb.

As a preliminary activity, a review of the models and mechanisms for irradiation creep proposed in the past will be carried out, as a guide for the simulation work. This review, based also on the evidence from the simulation work, should eventually lead to the design of experiments aimed at clarifying the role of the different possible mechanisms.

Both PPs share the long-term objective of deepening our understanding of the mechanisms behind materials degradation under irradiation, in the specific case of steels for GenIV applications, in order to set the bases for safer design rules and more reliable prediction of the lifetime of nuclear reactor core components.

[1] R.L. Klueh, A.T. Nelson, Journal of Nuclear Materials 371 (2007) 37
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[3] S.J. Zinkle, G.S. Was, Acta Materialia, 61 (2013) 735.

2. IOANIS pilot project (Ion irradiation as a neutron irradiation surrogate – Potential, challenges and limits)

The development and qualification of new structural materials for GEN IV applications require a profound understanding of the mechanisms of neutron damage and screening of a considerable number of materials to identify the most promising candidates. Both rely on comprehensive irradiation experiments with prototypic irradiation conditions.

The limited availability of suitable neutron irradiation facilities as well as costs and time expenditure of neutron irradiation experiments give rise to an interest in alternative irradiation sources which allow experiments involving a wide range of irradiation conditions. A number of energetic particles apart from neutrons, e.g. ions, protons and electrons, are used in irradiation experiments. However, by using a surrogate for neutron irradiation a transferability issue is introduced. In fact, a similar issue arises even for neutron irradiation experiments, due to limits in replicating the exact operation conditions, e.g. the neutron flux in case of accelerated in-core irradiations or the neutron spectrum in case of materials for fusion reactors.

The potential of ion irradiation to efficiently approximate neutron damage in structural materials and to serve as a tool for basic investigations and materials screening has long been recognized [1–3]. The attractiveness of ion irradiation is based on the short irradiation times to reach relevant damage in terms of displacements per atom (dpa) (hours and days compared to years), the avoidance of highly radioactive material, the comparably low costs and the relatively easy variability of irradiation parameters (e.g. irradiation temperature, fluence).

The transferability issue for ion irradiation with respect to neutron irradiation is primarily related to the displacement rate (dpa/s), which is several orders of magnitude larger in case of ion irradiation. In fact, increasing the dpa-rate (by using ions) does not simply accelerate the evolution of the irradiation-induced microstructure, but can lead to different results at the same irradiation temperature and dpa in specific cases. Approaches exist which try to compensate the effect of increasing dpa-rate by irradiation variable shifts, e.g. in temperature or dpa, [3,4]. However, these approaches reach their limits where complex initial microstructures and irradiation-induced microstructural changes with a variety of irradiation-induced features are involved.

Other factors contributing to the transferability issue include: the introduction of additional self-interstitials in case of self-ion irradiation [5-7], time dependence of the displacement rate, e.g. continuous or pulsed irradiation [8,9], differences in the cascade morphology and defect production efficiency [3] and gradients in defect concentrations due to displacement rate gradients and nearby free surfaces [10].

The issue of the transferability of ion irradiation results covers several aspects. As itt is impossible to address all aspects in the framework of one single project, in terms of irradiation parameters the present project will focus on irradiation temperatures from 200°C to about 450°C and on exposures up to about 10 dpa. The effects of dpa-rate, beam scanning and SIA implantation on irradiation-induced and irradiation-accelerated precipitation and on the formation of dislocation loops in ferritic/martensitic (F/M) steels will be addressed.

Two particular differences between the irradiation response of self-ion and neutron irradiations in Fe-Cr model alloys were recently observed:

- Dislocation loops showed a homogeneous spatial distribution after ion irradiation for all Cr contents investigated, while they were preferentially aligned along dislocation lines and grain boundaries in Fe-Cr alloys with 5 at% Cr or more after neutron irradiation [11,12].
- α'-phase particles were formed in Fe-Cr alloys with 9 at% Cr or more under neutron [13-16], but not under ion irradiation [11,12,17]

In contrast, the characteristics of the irradiation-induced CrNiSiP clusters [15-17] seem to agree for both types of irradiation. One aim of the pilot project is to address these and related issues by means of modelling and experiments.

A second transferability issue arises from the limited penetration depth of the ions, which is in the range of a few micrometres, and the non-homogeneous displacement profiles. They pose restrictions on the applicability of microstructural and mechanical characterisation methods which are traditionally applied to characterize neutron-irradiated (bulk) material and make it a challenge to obtain equivalent experimental information for ion-irradiated and neutron-irradiated material. APT and TEM can be readily applied to ion-irradiated material if the samples are extracted from a defined depth. However, the characterisation of the mechanical properties of ion-irradiated layers requires the application of nano-/micromechanical testing. Approaches based on NI exist [18-20], but need further qualification. The application of PAS and (GI)SAS to ion-irradiated layers remains challenging.

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3. ICAR pilot project (The influence of initial microstructure/carbon distribution to the swelling and hardening of irradiated FeCrxC alloys)

This pilot project is complementary to the IOANIS PP. Among the different alloying elements observed in ferritic/martensitic steels, this PP focuses on the role of C and on the influence of initial microstructure of 9%Cr steels and alloys to the defect properties formed after irradiation and their overall contribution to the degradation of the mechanical properties. Indeed, one of the main parameters which are responsible for the variation of the alloy microstructure and defect properties after irradiation is dissolved carbon distribution. Carbon easily segregates at dislocations and grain boundaries as well as it binds to neutron irradiation induced defects such as vacancy [1] and interstitial clusters and precipitates [2]. These nano-metric complexes obstruct dislocation motion, thereby increasing the hardening and consequently affecting the embrittlement.

Neutron irradiation and PIE of a variety of FeCrC alloys with different initial microstructures has been already performed within the European FP7/GETMAT project [3]. It was clearly observed that the properties of vacancy clusters depend on both Cr concentration and initial microstructure (depending on carbon content). Unfortunately, the FeCr alloys investigated in the GETMAT project did not have consistent microstructure which makes the analysis of the results difficult and uncomplete in terms of effect of microstructure and C content. Moreover, the segregation of dislocation loops at dislocations and their synergy with other defects as a function of the Cr and carbon content is still not resolved. For example the distribution of dislocation loops is found to be uniform in neutron irradiated Fe2.5Cr alloy, while in Fe5Cr, Fe9Cr and Fe12Cr alloys the dislocation loops are segregated at grain boundaries [3]. In addition, different loop distribution is observed as a consequence of neutron versus ion irradiation. Recent high dose ion irradiation experiments, on the other hand, show that swelling seems to be dependent on the type of microstructure: ferrite or F/M grains exhibit different swelling after irradiation [4].

This project aims at identifying the variation of the initial microstructure induced by varying Cr and carbon content in FexCrxC ternary alloys and to correlate the relevant features such as amount of ferrite to martensite phase, dislocation density, grain size, etc. to the mechanical properties of these alloys. In the second part of the project, the defect properties will be studied by focusing on the synergy between carbon, vacancy and chromium solute atoms in the clusters formed after neutron proton and ion irradiations, as well as the influence of the clusters for the changes in the mechanical properties. The focus is on hardening and swelling effects.

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4. MARACAS PP (Simulation of Model Alloys Representative of AustenitiC stAinless Steels)

Austenitic stainless steels are foreseen as cladding and structural materials for future generation IV reactors, in particular for the ESNII prototypes that are being designed now (ASTRID, MYRRHA, ALFRED and ALLEGRO). The reference alloys for the MYRRHA facility (LBE-cooled) and ASTRID prototype (SFR) are 316 L(N) austenitic steels for structures and components at high temperature and advanced austenitic steels (AIM1 or “15/15 Ti” steels) for cladding.

Structural materials will receive nearly no irradiation dose in ASTRID, except the lower grid of the upper core structure (UPC) which will receive a low irradiation flux with helium production due to transmutation. Even though the irradiation fluences are low, it is of prime importance for the 60-year design life demonstration to be able to predict the microstructure evolution that will alter its mechanical properties, in particular its creep resistance on the very long term.
On the contrary, cladding will receive very high irradiation fluences, so void swelling may appear and limit the lifetime of this component. Swelling resistance is the main reason for the choice of AIM1 steels instead of 316 steels. It should be noted that even with AIM1 alloys, however, swelling is such that at around 100 dpa the fuel will have to be removed from the reactor, whereas the burn-up is not complete. Swelling is a very complex phenomenon which is very sensitive to many parameters, such as dose rate, temperature, alloy starting state and alloy composition. In addition it does not evolve linearly with dose: it generally exhibits a transient or incubation regime with nearly no swelling but with microstructural evolution (notably in terms of dislocation microstructure), followed by a steady state regime where it evolves linearly with the dose. Extending the incubation regime is thus a key issue to increase the lifetime of cladding.

For both structural materials and cladding materials it thus appears crucial to understand the microstructural evolution, especially at low doses. Major elements are known to have an effect on the duration of the incubation regime [1], with for example very large effects of Ni when the content is changed from 30 to 35 wt%. Such effects are still badly understood and no model exists to reproduce them. Concerning minor elements (C, P, Si, Ti, etc.), they play a major role on swelling and more globally on the whole microstructure evolution. They can either act when they are in solid solution (by modifying the diffusion of self-defects, dislocation biases, dislocation motion, etc.) or as part of precipitates. Their multiple effects on the incubation regimes are very difficult to disentangle, especially when the number of solute elements is high as in commercial steels.
The goals of this PPP are twofold:

- First, to gain a better understanding of the thermodynamics (phase diagram, point defect formation energies) and kinetics (diffusion properties, segregation, ordering) under irradiation in binary and ternary model alloys.
- Secondly, to better understand the microstructure evolution at low dose in pure Ni with the addition of a limited number of minor elements. We will choose Ti as a substitutional dilute solute and C as an interstitial impurity. These elements are essentially known to reduce swelling but their precise role and their synergetic effect on the microstructure are still not firmly explained.

[1] W. G. Johnston *et al.*, J. Nucl. Mater. **54**, 24 (1974)

5. SLIPLOC PP (SLIP LOCalization in irradiated steels and consequences on mechanical damage)

This project aims at **predicting deformation localization** occurring during tensile or cyclic loading of pre-irradiated steels. The project concerns the main steels used in fission reactors of all generations (ferritic-martensitic and austenitic stainless steels).
Slip localization occurs in a wide range of pre-irradiated metallic materials subjected to tensile or cyclic loading.
Slip localization and related micro-structure evolution has been extensively observed to occur at the grain scale, particularly in Faced-Centred Cubic (FCC) metals and alloys, but also in Body-Centred-Cubic (BCC) and Hexagonal-Close-Packed (HCP), subjected to post-irradiation deformation [1]. Slip localization has been observed at dose as low as 0.01 dpa (copper, copper alloys) and for temperature as high as 300°C (austenitic stainless steels and ferritic steels) and probably above. **The key point is that plastic deformation in a slip band is at least ten times greater than in the matrix, leading to series of generally deleterious consequences** [see a review in 2]. It should finally be noticed that slip localization inside thin slabs is observed in other conditions, for instance tensile or cyclic deformation of metals and alloys leading to crack initiation too (see a review in [3]).
Even if the mechanisms of slip band formation differ in some details, numerous common features are evident:

- Gliding dislocations meet obstacles (radiation-induced defects as small loops, precipitates, solid solution atoms...);
- They react with these obstacles by various ways such as sweeping, drifting, cutting and absorption processes;
- These mechanisms lead to the formation of thin bands almost free of obstacles, where dislocations glide easily, leading to strong slip localization.

A **multiscale modelling** approach is applied to predict slip localization features and consequences in terms of mechanical damage (necking, intergranular damage occurring in both inert and corrosive environments). At the lowest scale, molecular dynamics will allow a fine characterization of dislocation – irradiation defects interactions, completing the existing results, as well as the evaluation of radiation-induced loop and chemical segregation around dislocation lines. **Discrete Dislocation Dynamics** computations together with a continuum modelling based on dislocation and defect evolution equations will be carried out to predict the formation of clear bands and the induced slip localization. Finally, higher scale modelling based on non-convex potentials, polycrystalline homogenisation, necking theory or grain boundary fracture criteria will permit the **prediction of the macroscopic behaviour** of the pre-irradiated steels and **how slip localization leads to damage and fracture**. Each computation level provides inputs used at the higher level. And each modelling will be assessed thoroughly by various experimental observations and measurements carried out at the corresponding scale. Tomography atom probe (TAP), in-situ TEM, TEM as well as SEM and Electron Back Scattered Diffraction (EBSD) will be used.

Our goals are a better understanding and modelling of slip localization in irradiated metals and alloys and its consequences.

[1] Neuhaüser, H., 1983. Slip line formation and collective dislocation motion. Dislocations in Solids. Edited F. R. N. Nabarro, Vol. 6, pp. 319.
[2] Sauzay, M. and Vor, K., 2013, Influence of plastic slip localization on grain boundary stress fields and microcrack nucleation, *Eng. Frac. Mech*., 110, 330
[3] Sauzay, M. and Kubin, L., 2011, Scaling laws for dislocation microstructures in monotonic and cyclic deformation of fcc metals, *Prog. Mat. Sci*., 56, 725.

6. MOSEL PP (Modelling Steel Embrittlement by heavy Liquid metals)

The objective of this Pilot Project Proposal is to contribute to the comprehension of the physics and the microstructure evolution governing the liquid metal embrittlement (LME) of steels exposed to heavy liquid metals (HLM).
LME refers to various different phenomena that take place when a ductile metal in contact with a liquid metal shows an unusual and unpredictable brittle behaviour if stressed in tension, compared with the tensile behaviour in air. LME occurs in a wide range of specific solid-liquid metal combinations and is strongly affected by the chemical compositions of the solid and liquid metals.
A large amount of experimental data from mechanical testing in liquid lead alloys and, to a smaller extent, in pure lead environments has been obtained during the last decades in the context of the former FP7, FP5 and FP6 projects and in support of the MEGAPIE international initiative. Ferritic/martensitic steels are reported to suffer from this issue, and thanks to the extensive work done, the features of the phenomenon are at least qualitatively delineated.
Austenitic steels seem to be much less affected by this issue, at least at temperatures below 400°C, nonetheless as demonstrated in the FP7 MATTER project, the use of some type of filler material to reduce the susceptibility to hot cracking, can lead to a delta ferrite contents up to 5% in the welds. LME could have a serious impact on the mechanical properties of welded joints of austenitic steels exposed to HLM. The role of unstable austenite having a martensitic transformation under mechanical strain is also a possibility that would render austenitic steels more susceptible to LME.
A clear understanding of the mechanisms behind HLM LME is still missing as well as a model to rationalize the whole body of experimental data. It is widely recognized that the main source of uncertainty is related to the complexity of the phenomenon and to the difficulties in controlling the experimental details that make difficult to discriminate the processes relevant to LME from those that are not.

Atomistic modelling of the solid-liquid interfaces and grain boundaries in the presence of HLM and a targeted experimental campaign on model systems can contribute to the achievement of a better understanding about the interactions and processes at the origin.

This project proposes an approach where the development of models will be used in synergy with targeted experiments and advanced microstructural characterizations. The theoretical effort will require the development of reliable models of molten lead alloys, models of iron and iron chromium alloys interfaces in contact with the liquid metal with and without the application of external stress fields. The theoretical work will be integrated by mechanical characterizations and wetting experiments on model systems and under careful control of the chemistry.

7. MOLECOS PP (MOlten LEad and lead bismuth COrrosion of Steels)

The objective of this project is to obtain a basic understanding of the processes involved in the corrosion of steels by molten lead and lead bismuth. Corrosion represents a critical challenge in the use of heavy liquid metals (HLM) as coolants for the realization of Gen IV reactors and concentrated solar power systems.

A controlled surface oxidation (Active Oxygen Control, AOC), obtained maintaining a low concentration of oxygen in the molten metal, has proven to be an effective mean to promote the formation of a self-healing oxide film on the steels surface, so reducing steel corrosion and coolant contamination.

On the other hand it has been shown that above temperatures around 450~500°C, depending on the steel considered and on the experimental conditions, the technique is not effective and severe corrosion attacks are observed. The development of a chromium rich oxide layer on the steel surface, that acts as physical barrier to further oxidation in most environments, is not effective in HLM at high temperature. The feature responsible for the increased corrosion rate is an unusual oxygen diffusivity trough the oxide scale, whose mechanism is still not understood. A research line that received little or no attention by the research community is that the enhanced corrosion observed at high temperatures in those environments can be associated with the chemical interaction of the steels with the coolants via the formation of complex oxides. The precipitation of defective structures permeable to oxygen or low melting compounds can justify the enhanced oxygen diffusion and enhanced corrosion.

Investigate this promising hypothesis involves the careful characterization of the composition and crystallographic structure of the oxidation products and the knowledge of the properties of the phases that may form. The main obstacle is the unavailability of thermo-physical and structural data for the steel-HLM-Oxygen system. To try to fill this lack, targeted corrosion experiments, carried out with an accurate control of the chemistry and advanced characterization techniques, coupled with a computational approach are proposed. In particular, the theoretical approach will contribute to estimate the data not available in the literature by means of codes based on the minimization of the Gibbs free energy.

The chemical interaction of the steels with the coolants and impurities, coming from the dissolution of the steels or introduced for conditioning purposes, plays a key role also in the implementation of the AOC coolant chemistry control systems. Atomistic modelling will be used to gain important information about the solubility and diffusion data, fundamental to understand the interaction of the dissolved metallic impurities (Fe, Ni, Cr, Mn) with oxygen and hydrogen in the HLM. The results of the calculations will be used for the interpretation of a dedicated experimental campaign and for a critical review of the literature data.

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[2] Walter M. F. Fabian, Accurate thermochemistry from quantum chemical calculations?, Monatsh. Chem. 139 (2008) 309

[3] G. Eriksson, "Thermodynamic studies of high temperature equilibria", Acta Chem. Scand. 25 (1971) 2651

III. Participants and human resources

Participants Name		Short Name	Country
Commissariat à l'Energie Atomique et aux Energies Alternatives		CEA	France
	Electricité de France Recherche & Developpment	EDF R&D	France
	Université de technologie de Belfort-Montbélliard	UTMB	France
Conseil National de la Recherche Scientifique		**CNRS**	**France**
Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas		CIEMAT	Spain
	Universidad de Alicante / Universitat d'Alacant	UA	Spain
	Universitat Politècnica de Catalunya	UPC	Spain
Consiglio Nazionale delle Ricerche		CNR	Italy
Research centre REZ		CV REZ	tchek republic
Ente Nazionale per l'Energia e l'Ambiente		ENEA	Italy
	Politecnico di Milano	POLIMI	Italy
Helmholtz-Zentrum Dresden-Rossendorf		HZDR	Germany
Joint Research Centre – Institute of Energy and Transport		JRC-IET	EU
Karlsruhe Institute of Technology		KIT	Germany
	Materialprüfungsanstalt Universität Stuttgart	MPA	Germany
Royal Institute of Technology		KTH	Sweden
Nuclear Research and consultancy Group		NRG	The Netherlands
Paul Scherrer Institute		PSI	Switzerland
	ETH Zürich	ETHZ	Switzerland
Studiecentrum voor Kernenergie • Centre d'Etudes de l'Energie Nucléaire		SCK•CEN	Belgium
	Université libre de Bruxelles	ULB	Belgium
	Institute of Physics Zagreb	IFZ	Croatia
Slovak University of Technology		STUBA	Slovakia
UK Engineering and Physical Sciences Research Council		UKERC	United Kingdom
	Middle east technical university	METU	Turkey
Technical Research Centre of Finland		VTT	Finland
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