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PROJECT FINAL REPORT

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List of acronyms used in this report

2D: 2 Dimensions (x,y) plane
3D: 3 Dimensions (x,y,z) space
AFTM: Advanced Fracture Toughness Model
APT: Atom Probe tomography
AKMC: Atomic Kinetic Monte Carlo
BCA: Binary Collision Approximation
BCC: Body Centred Cubic
BWR: Boiling Water Reactor
BF: Bright Field
CH: Cahn-Hilliard
CKMC: Cellular Kinetic Monte Carlo
CRPs: Cu-rich precipitates
CZM: Cohesive Zone Model
DD: Dislocation Dynamics
dpa: Displacement per atom
EAM: Embedded Atom Model
EC: European Commission
EIS: Electrical impedance spectroscopy
E&RC: Evaluation and Review Committee of the project
FCC: Face Centred Cubic
FEGSTEM: Field Emission Gun Scanning Transmission Electron Microscope
FE: Finite Element
FL: Franck Loops
FP: Framework programme
GB-RIS: grain boundaries suffering radiation-induced segregation
GGA: Generalised Gradient Approximation
IASCC : Irradiation assisted stress corrosion cracking
IGSCC : Inter-granular stress corrosion cracking
IAEA: International Atomic Energy Agency
LWR : Light Water Reactor
MD: Molecular Dynamics
MFRT: Mean Field Rate Theory
MSM: Multi-scale simulation modeling
MMC: Metropolis Monte Carlo
MNPs: Mn-Ni(-rich) precipitates
MS: Molecular Statics
NEA: Nuclear Energy Agency
OKMC: Object Kinetic Monte Carlo
PAS: Positron Annihilation Spectroscopy
PAW: Plane Augmented Wavefunction
PD: Point Defects
PM: ParaMagnetic
PIM: Pair Interaction Model
PKA: Primary Knock on atom
PTS: Pressurised Thermal Shock
PWR: Pressurised Water reactor
RPV: Reactor Pressure Vessel
RIS: Radiation Induced Segregation

SCC: Stress Corrosion Cracking

SCMF: Self-Consistent Mean Field theory

SF-PDM: Spinel, Field-Point Defect Model
SIA: Self Interstitial Atoms
SIPA: Stress-Induced Preferred Absorption of defects
SQS: Quasi-Random structures
SP: Sub-Project
SS: Stainless Steel
SSRT: Slow Strain Rate Tests
TEM: Transmission Electron Microscopy
TIP: Thermodynamics of Irreversible Processes
UG: User's Group
WBDF: Weak Beam Dark Field
WP: Work package
XPS: X-ray photon spectroscopy

Content

Executive summary

Since 2002, the European Commission (EC) has been supporting (FP6-PERFECT and FP7-PERFORM 60) the development of simulation models based on multi-physics and multi-scale approaches, to be able to understand the origin of the onset of reactor pressure vessel (RPV) steel embrittlement and the susceptibility of its internals to Irradiation Assisted Stress Corrosion Cracking (IASCC). Indeed, the safe operation of a nuclear reactor depends on our capability of maintaining the integrity of these important components.

The main aim of the commonly deployed effort is to develop future tools useful for industrial and research projects, related to the prediction of material behaviour under nuclear power plant operating conditions, by means of:

- A sharp understanding of the physical phenomena and interaction between them (experimental tests, observations).
- An accurate definition of the several blocks needed for the modelling– ˝localisation strategy˝.
- The simulation (as physically as possible) of the observed local phenomena and interaction between them, using powerful numerical tools to bridge and homogenize in time and space – ˝homogenization strategy˝.
- The validation of the tools using representative in-pile experiments.

The development of multi-scale numerical tools able to simulate the effects of irradiation on materials microstructure, flow & fracture behaviour, SCC sensitivity, is a long term endeavour and requires among others:

- Development/improvement of appropriate mechanistic models at different levels of physics and engineering,
- Extension beyond the actual state of knowledge in several scientific fields.
- Extensive experimental and theoretical validation of the models at the appropriate scale.
- Efficient and correct link between the different kinds of models bridging various space and time scales

The collaborative project PERFORM 60 officially started on March 1st, 2009 for duration of 48 months and was extended by 10 months until December 2013. It was performed by a European consortium comprising twenty organizations (3 utilities, 1 constructor, 9 national research centres and 6 universities) from 7 different countries.

PERFORM 60 is based on two technical sub-projects, namely Reactor Pressure Vessel (SP-1) and Internals (SP-2). In addition, a Users' Group and training scheme have been established to allow representatives of constructors, utilities and research organizations from all over the world to participate actively in the process of appraising the limits and potentialities of the developed tools as well as their validation against qualified experimental data. In fact, a close collaboration with an international user group composed by 15 organisations originating from USA, Japan, Russia, Korea, UK, Sweden, Argentina, Finland and Switzerland, has been established in the course of the project.

Furthermore, a significant effort has been made to make young researchers in the field of materials degradation in the nuclear field aware of the potential value of multi-scale modelling, and to disseminate the results of PERFORM 60 among the different partners in international conferences, peer-reviewed journals and via a dedicated web-site.

This work has allowed the EU's nuclear industry to take a leading position in the field of numerical simulation for residual lifetime prediction, to make discoveries and obtain insight into the physical behaviour of nuclear materials, to optimize and facilitate synergies among research centres, universities and industries using relevant installations (e.g. high performance computers, hot cells, …) and expertise in a wide range of disciplines.

Project context and main objectives

In nuclear power plants, reactor materials may undergo degradation in physical and mechanical properties due to severe in-service irradiation. In fact, materials subjected to irradiation with energetic particles (such as neutrons …) suffer significant changes in their microstructure followed by drastic modifications of many physical and mechanical properties. Indeed, due to the harsh operating environment combining high temperature, intense radiation flux and aggressive chemical reactivity, the safe and economic utilization of nuclear power has raised tremendous challenges for materials used in current and future fission nuclear reactors. Therefore, understanding and predicting radiation effects is vitally important to ensure the reliability of existing materials and to improve the development of new generations of advanced structural and functional materials for energy production and other applications.

At the moment, most investigations into the behaviour of materials used in nuclear power plants are conducted by irradiating specimens, either in surveillance capsules, or in test reactors, and subsequently performing mechanical tests and (to a lesser extent) micro-structural characterisations in hot cell facilities, where the samples are handled remotely and safely. Pressure vessel surveillance capsules are positioned closer to the core than the vessel wall and thus receive a slightly higher flux. The specimens therefore reach higher fluence more quickly than the vessel wall, and their periodic testing enables the evolution of the mechanical behaviour of the wall to be predicted. In material test reactors, specimens are irradiated at much higher fluxes, in conditions otherwise similar to those experienced in service, so as to reach the same fluences expected at the end of the service life and beyond in a much shorter amount of time. However, the number of capsules available for evaluating the performance of the pressure vessel materials beyond the originally envisaged service life is limited. Furthermore, this procedure is expensive, which limits the number of tests that can be conducted and the irradiation conditions that can be explored. Moreover, in the last couple of decades the number of operating test reactors and hot cell laboratories has been decreasing steadily world-wide. Stricter safety requirements have made managing such facilities more and more expensive and even the relevant expertise is slowly disappearing. Thus, the amount of data available for long-term predictions is reaching its limit and alternative means for evaluating the behaviour of materials under irradiation are needed. At present, long-term predictions of the lifetimes of nuclear components are made using semi-empirical correlations that provide trend curves. These correlations are based on the available databases, which include surveillance data and also data from materials test reactors. However, their validity is limited to the parameters range of the data and they are most of the time strictly confidential. Thus, to allow a rigorous implementation of this aging phenomenon both in the long term operation and in the design of a nuclear power plant, it is of paramount importance to develop physically based models.

The macroscopic behaviour of materials is necessarily always the result of processes at the atomic scale. However, in many instances, the discrete atomic nature of materials, and the fact that their chemical composition may change locally, is neglected for modelling purposes and continuum approaches can be in practice very effectively used. The thermo-mechanical behaviour of plant components, also for nuclear applications, is typically modelled using finite element (FE) techniques. With these techniques, the continuum equations governing elastic and plastic behaviour, coupled if needed to heat or even mass transport equations, are solved with appropriate boundary conditions. The core of the methodology in this case is constituted of phenomenological constitutive laws, which provide the relationship between, for example, stress and strain for each phase, or between temperature gradient and heat flux, or between concentration gradient and mass flux. The effective physical parameters that appear in these laws, such as elastic moduli, thermal conductivity or diffusivity, must be known. Within this continuum approach, the main concern is that the phenomenological constitutive laws and the parameters that appear in them should be representative of the actual properties of the real material, which is not a continuum. If proper constitutive laws are given, several methodologies are traditionally used to compute, for example, the macroscopic stress-strain response of the material and therefore its effective plastic behaviour. Refined calculations can be performed using numerical homogenization methods with FE calculation of microstructures.

In the case of radiation effects in solids, however, no *physically-grounded* model can completely ignore the atomic nature of materials and the presence of different chemical species, because most processes of importance are strictly atomic (or even nuclear) in nature. The development of continuum *physical* models is possible, as long as sufficient information translating the effect of atomic, nano- and micro-structure is brought into the constitutive laws. Continuous progress in physical understanding of radiation damage and in computer technology has made it possible to develop multi-scale numerical tools capable of simulating the effects of neutron irradiation on mechanical and corrosion properties of reactor materials.

A first step towards the establishment of this new methodology has been successfully reached in the European scientific community created around the FP6 PERFECT project. Based on the achievement and the roadmap established with this initial project, the European Commission decided to support the collaborative project PERFORM 60, with the overall objective to further develop the multi-scale modelling tools capable of predicting the combined effects of irradiation and corrosion on internals (austenitic stainless steels) and of radiation induced embrittlement of reactor pressure vessel components (low-alloy bainitic steels).

To reach this overall objective, the proposed work was divided in several milestones such as:

(i) The production of more advanced versions of RPV-module dedicated to simulate/predict the evolution of the microstructure under irradiation and the resulted hardening, together with an improved Fracture Toughness Module to model/predict the irradiation effect on the brittle to ductile transition temperature (ΔT) (see figure 2) of the reactor pressure vessels of PWRs and BWRs for durations up to 60 years;

(ii) A platform of simulation tools to integrate and chain all the modules developed (based on the same concept developed within FP6-PERFECT project) to couple various physical phenomena, such as, corrosion and irradiation effects on reactor internals in PWRs and BWRs;

(iii) Experimental validation and model qualification using industrial plant data and results of existing or new laboratory experiments (including non EU sources) as necessary. In addition, other means of validation such as benchmarking with existing qualified calculation codes were considered.

(iv) Establishment of a Users' Group to test the newly developed modelling tools in a number of benchmark exercises with a view to their qualification, in close links with the NEA and/or IAEA databanks and activities.

In practical terms, the project is based on three sub-projects: i) Reactor Pressure Vessel (SP-1), ii) Internals (SP-2) and iii) Users' Group (SP-3). The interaction between them is illustrated in Figure 1.

The context and the objectives of these technical sub-projects are described in the following:

Sub-Project 1 “Reactor Pressure Vessel”

Ferritic pressure vessel materials (generally low-alloy bainitic steels) are subject to neutron irradiation during their operational lifetimes and, if damage doses reach only ~ 0.2 dpa at the end of life (40 years), the irradiation-induced shift in the brittle to ductile transition temperature for current RPV steels should not exceed typically 100°C, as illustrated schematically in Figure 2, in order to avoid any brittle fracture of the RPV during the various transients or emergency cooling. For this level of damage, the mechanisms are understood reasonably well, but, in the case of an end of life of more than 40 years, different questions arise:

- Does accumulation of more than 0.2 dpa induce other damage mechanisms (for example: segregation of phosphorus to the grain boundaries or development of new phases after a certain incubation time)?
- What is the effect of temperature (~320°C) for a duration of more than 40 years?

The research activities described under SP-1 “Reactor Pressure Vessel” build on previous actions in project PERFECT, with the following objectives:

- Produce an Advanced Fracture Toughness Module (AFTM) based on development and integration of the multi-scale simulation tools RPV-2 (→RPV-n) and the Fracture Toughness Module created in FP6 project PERFECT to simulate the irradiation degradation on reactor pressure vessels of PWRs and BWRs for durations up to 60 years.
- Benchmark the numerical results from the AFTM and compare these, where appropriate, with existing analytical methods and data (e.g. via the NEA and (or) IAEA databanks).
- Provide additional experimental validation and model qualification for the AFTM using industrial plant data and results of existing or new experiments (including non-EU sources) as necessary.
- Build the AFTM based on a strong interaction with the End Users’ Group (SP-3) of PERFORM 60.

All the developed simulation codes are integrated with the primary objective to collect in a multi-scale modelling numerical platform the scientific and technical advances performed within SP-1 "RPV". For this purpose, the PERFORM 60 numerical platform architecture, structure and development language were developed based on continuity with the PERFECT project numerical platform. The existing set of codes and knowledge already available for the scientific community in the existing platform was optimised and enriched with new physical schemes and computational tools.

Furthermore, it was intended to ensure and maintain a high level quality process for the integration of the scientific and technical products developed by the research teams involved in PERFORM 60. With this aim, the documentation and validation of the computational tools integrated in the numerical platform is seen as an essential element allowing the European scientific community to exchange information on the state-of-the-art and on their recent advances and developments.

Sub-Project 2 “Internals”

The internal components of light water reactors are fabricated from austenitic stainless steel and surround the fuel elements and ensure their positioning and cooling by supporting them and guiding the coolant flow, illustrated in Figure 3. The internals are exposed to intense neutron irradiation (over 1dpa per year, depending on the reactor design), mechanical and thermal stresses and the corrosive action of the high temperature water coolant. This exposure may lead to several degradation mechanisms, limiting the useful lifetime of the internal components. The three main degradation mechanisms under consideration are: irradiation assisted stress corrosion cracking (IASCC), irradiation creep and irradiation induced swelling.

For the light water reactors, currently in operation, no systematic data are available on the long term behaviour of the materials used for the internal components. This is due to a number of reasons:

- The lack of planned surveillance programmes for internals (as opposed to the reactor pressure vessel);
- Insufficient experimental development and optimisation (as is the case for fuel cladding materials);
- Insufficient information obtained from extracted components.

The available knowledge on degradation of the internal components of LWRs originates mainly from the analysis of extracted components or from tests on specimens, irradiated in test reactors (mostly under somewhat different conditions than those in the operating LWRs). Due to the difficulty and cost of these tests on irradiated materials, the scope of research programmes has been limited so far, bringing mainly only qualitative understanding of the degradation phenomena and sparse/partial parameterisation of the observed degradation behaviour against the large number of variables to be considered.

From this short discussion, a clear need emerges to understand and parameterise the irradiation induced degradation mechanisms, relevant to internals in LWRs. Therefore, the sub-project on austenitic stainless steel internals focused on producing models that are able to describe/simulate the occurrence of Irradiation assisted stress corrosion cracking (IASCC) under relevant conditions, by developing and qualifying a set of simulation modules able to provide mechanistic and physical insights on this degradation phenomenon over relevant dose, temperature and environmental conditions.

IASCC involves the highest degree of complexity in the multi-physics chain, as it integrates aspects of radiation induced microstructure modifications, environmental interactions and mechanical behaviour. Within the limits of the project resources and in accordance with the expression of interest of the potential end-users, the option has been taken to focus the efforts on predicting crack initiation. For parameterisation and validation, the initiation of IASCC in irradiated SS type 316 stainless steel was taken as the reference case. In order to address different physical aspects and to integrate inputs from the underlying WPs, the sub-project produced models at different scales:

- Component-specimen scale: a statistical model has been developed, predicting the distribution of cracks initiated as a function of time, load and material properties. This scale relied on the lower scale models for parameterisation beyond purely empirical data fitting.
- Continuum scale ("representative volume element"): at this scale, deterministic models have been formulated, integrating the mechanical and chemical contributions to crack nucleation and growth.
- Aggregate scale: at this scale, physics based models have been chained in order to predict the occurrence of elementary cracking events by integrating the description of the mechanical behaviour of the irradiated material with the corrosion and oxidation behaviour of the grain boundaries.

The developed tools were assembled from a chain of modules, each describing a single physical phenomenon. The validation of the models has been performed to a maximum extent for every module within the final products, in order to estimate the contribution of each module to the general uncertainty on the prediction. Although some of the verification experiments were carried out on model materials or calculations, reference to industrially relevant materials and conditions was made to a maximum extent.

Sub-Project 3 "Users' Group"

The scientific approaches developed in the SP-1 and SP-2 sub-projects to model the behaviour and degradation mechanisms of reactor pressure vessel (irradiation embrittlement) and internals (IASCC) materials are very innovative both because of the techniques used for numerical simulation and of the challenge to derive the macroscopic component behaviour from the microscopic evolutions of the material.

Therefore, to fully reach the goals of the project, a complementary work was done through a Users' Group with the main objectives: i) to assess the developed modelling with industrial data and ii) to share the knowledge and modelling approach improvements among the European nuclear community and beyond. This work included the publication of the state of the art with a critical evaluation of existing tools and approaches in a 60 years operation context, a collection of experimental reference data and a proposal of industrial applications, and a final evaluation of simulation tools through their applications to collected reference data and applications. A final workshop was organized at the end of the project, for a final evaluation of all end products with identification of missing gaps.

Within the framework of this Users' group, the dissemination of the created knowledge during the project was broadening to include not only European nuclear community but also outside the European Union. The created knowledge includes modelling approach improvements, new modelling tools and qualified experimental data both from the examination of in-service components and laboratory experiments (see the section on dissemination activities).

Main Scientific and technical results

I. Modelling of radiation damage (embrittlement) on reactor pressure vessel steel behaviour: SP1

Based on the multi-scale approach adopted within the FP6-PERFECT project, illustrated in Figure 4, that enabled the simulation of the evolution of irradiation-induced microstructural changes and the degradation of mechanical properties using the end-products RPV-2 and Toughness, respectively, the FP7 -PERFORM 60, adopted a top down approach to gain a better physical insight into the behaviour of more realistic RPV materials. The content as well as the chaining of these 2 end-products is illustrated in Figure 5.

This SP was organized, in 4 work packages enabling the development of a robust framework to improve, develop and possibly integrate the appropriate models build at each physical scale. In the following sub-sections, firstly, the main development concerning models, shown in Figure 5a, for the prediction of the microstructural evolution of model alloys is described. Thereafter, a succinct reporting on the new models that have been established and validated to describe both the flow behaviour and the irradiation hardening of RPV steel is given. Thirdly, the most advanced fracture toughness models investigated within this SP are described (figure 5b). Finally, the numerical integration of the different end-products in the PERFORM 60 platform is detailed (chaining of the models of figure 5a with those in 5b).

I.1. Modelling of the microstructural evolution of RPV steels under irradiation

Detailed microstructural examinations of irradiated RPV steels and relevant model alloys performed over the last twenty-five years, using especially atom probe tomography (APT), have clearly shown that solute clusters formed under irradiation have complex chemical compositions. Depending on RPV steel composition, two different types of solute aggregates can be the cause of hardening/embrittlement after irradiation, namely Cu-rich precipitates (CRPs) and Mn-Ni(-rich) precipitates (MNPs). The fact that Cu is generally found in both families, although in different relative amounts, has been interpreted as evidence that this element is in all cases the catalyst of precipitation, but the possibility of forming Mn-Ni precipitates (MNPs) in low Cu steels was put forward in the 1990’s, deducing that, also in high-Cu steels, at high doses, once most Cu is precipitated, it might become possible to trigger the precipitation of MNPs. This consideration suggested for MNPs the expression “late blooming phases”, which is now the most widespread term. The challenge is to be able to establish whether or not these clusters can be precursors of these so-called “late blooming phases”. This phenomenon, is defined as an onset of radiation induced embrittlement after a certain dose, and has been reported to become eventually detrimental for the integrity of RPV if operating for periods longer than 40 to 60 years.

Atom-based multi-scale modelling was developed essentially either for pure metals under irradiation or for simple alloys such as Fe-Cu within PERFECT project. The major challenge of the PERFORM 60 project was to introduce a physical description at the atomic scale of the effect of the major alloying elements (e.g. interstitials like C, and substitutionals such as Cu, Ni, Si, Mn) in the evolution of the microstructure, on the hardening and on the loss of fracture toughness after irradiation.

The work performed during this work package (WP) aimed to develop physical models that describe the nanostructure evolution under irradiation in body-centred cubic (bcc) Fe model alloys, with increased complexity- starting from pure Fe, up to FeNiMnSi(Cu) approaching therefore the composition of RPV steels stepwise. The developed predictive tools enabled the quantification of nano-structural features, in terms of their density and size distribution. These are clusters of vacancies, self interstitial atoms (SIA) as well as solute atoms that grow into voids, dislocation loops and precipitate, respectively.

The first major task was to acquire a large set of density functional theory (DFT) data on configuration energies of point-defects and their clusters, as well as migration energies in pure α-Fe, including the effect of solute-defect interaction, both for substitutional (Cu, Ni, Mn, Si, P) and interstitial (C, N) solute atoms has been produced, in order to help develop adequate interatomic potentials for multi-component alloys or to set up the interaction energies needed to model the long term behaviour using Monte Carlo techniques or mean field theories.

In the course of the project, a scientific breakthrough has been achieved by exploring a new formalism (based on Embedded Atom model) to create multi-components interactomic potentials that are not only compatible with the main physical properties of the alloy (i.e. elastic modulus, point defect formation, ...) but also with the thermodynamical stabilities of alloys as a function of composition and temperature. Using these advance schemes, new potentials have been developed for Fe-C, FeCuC, FeMn, FeNi and FeNiMn.

Each of the developed potentials has been validated against the existing experimental data, available in the open literature, in terms of formation and migration energies for point defects and solute-point defect clusters. But, the most important effort was undertaken to develop higher scale models (longer time scale, and larger simulation volumes) in order to be able to validate the output directly with the experimentally observed behaviour of neutron irradiated alloys.

Many cases have been studied, as it can been seen from the various publications listed below. In this report, only 3 examples are described hereafter to illustrate the successful achievements made.

Example 1: microstructure evolution in FeCuC

Firstly, a model for simulating the nanostructural evolution under irradiation in Fe-C alloys has been developed using a physical description of the properties of vacancy and self-interstitial atom (SIA) clusters, based on the selection of the latest data from atomistic studies and other available experimental and theoretical work from the literature. The effect of carbon on radiation defect evolution has been understood in terms of the formation of immobile complexes with vacancies that in turn act as traps for SIA clusters. It is found that this effect can be introduced using generic traps for SIA and vacancy clusters, with a binding energy that depends on the size of the clusters, also chosen on the basis of previously performed atomistic studies.

A number of sensitivity studies to explore the effect of parameters on the model, have been performed. These include effects such as carbon content in the material, represented by generic traps for point defects, the importance of traps, the size dependence of traps and the effect of the dose rate. It was shown that (Figure 6), in order not to feel the effect of C, very small concentrations need to be reached, which is unlikely to be achievable in reality, both because of the difficulty of producing ultra-high-pure iron and because of the unavoidable C contamination during the performance of irradiation experiments. On the other hand, above a certain concentration there is a kind of saturation of the effect of the presence of C in the matrix. This explains why experimentally it is very difficult to appreciate the effect of the presence of C on the nanostructural evolution under irradiation in Fe-C alloys.

Quite clearly, this model is a good reference as it was proved suitable to reproduce the results of low (<350 K) temperature neutron irradiation experiments (see Figure 7). Therefore it was used as the starting point to include the effect of substitutional solute atoms, such as Cu, on the one hand, and Mn and Ni, on the other.

The next step has been the introduction of Cu in terms of a concentration of solute atoms that interact with vacancies forming Cu-vacancies complexes, governed by laws for their stability and mobility that were previously calculated by means of (atomic kinetic Monte Carlo (AKMC) models. Encouraging results have been obtained in terms of density and size of Cu precipitates formed under irradiation at RPV operational temperature, see Figure 8, when compared with the experimental results obtained from the investigation of the same alloy using many experimental techniques such as positron annihilation spectroscopy (PAS), small angle neutron scattering (SANS) and tomographic atom probe (APT) as it was performed during the FP6 project PERFECT. One of the key assumptions has been to impede the recombination of vacancies when they are surrounded by Cu atoms in clusters that are sufficiently large to be seen as hollow precipitates.

Example 2: microstructure evolution in FeNiMn

The purpose of this activity was to calculate sets of parameters relevant for object kinetic Monte Carlo (OKMC) simulations of radiation-induced nanostructural changes in model FeMnNi alloys. These models are ultimately intended to describe the formation of MnNi clusters under irradiation, according to the correct physical mechanism. Atomistic studies performed within the project and educated guesses based among other things on published density functional theory (DFT) data suggest that, Mn and Ni cause a strong reduction in the mobility of SIA and vacancy clusters and are transported in an Fe matrix by single point-defects: the key mechanism leading to the formation of solute clusters, by segregation on point-defect clusters (heterogeneous nucleation).

In addition, it has been shown, experimentally within the project that the presence of Ni and Mn in Fe has three effects, namely:

- Suppression of the formation of vacancy clusters and nanovoids as compared to Fe-C;
- Suppression of the formation of visible loops: their density being one order of magnitude less and their mean size about half as compared to Fe-C.
- Appearance of an important population of Ni-Mn clusters at high enough dose (>0.1 dpa): that reaches a density of almost 10^{24} m^{-3}, with mean size around 1.5 nm.

To account for the above observation, it was necessary to develop a new OKMC model, called (MATEO) to allow solutes (Ni and Mn) to be explicitly introduced and transported by defects. The results obtained from these simulations of the alloy Fe-0.7%Ni-1.2%Mn at 563 K up to 2dpa, selected as it can be compared with the experimental results obtained in the framework of the FP6-PERFECT project are illustrated in Figure 9, as a snapshot in a volume comparable with that observed in atom probe examinations, $11\times11\times70$ nm^3. The main difference from an atom-probe output is that here also vacancies and SIAs, invisible to atom probe, are shown. It can be observed that NiMn clusters are clearly formed everywhere in the simulation box.

The results concerning both density and mean size of Mn-Ni clusters are in excellent agreement with the experiment, as shown in Figure 10.

Example 3: microstructural evolution in FeNiMnCu

In this work, an atomistic kinetic Monte Carlo (AKMC) model parameterised on electronic structure calculations data has been developed and used to study the formation and evolution under irradiation of solute clusters in Fe-MnNi ternary and Fe-MnNiCu quaternary alloys.

Two populations of solute rich clusters have been observed which can be discriminated by whether or not the solute atoms are associated with self-interstitial clusters. Mn-Ni-rich clusters are observed at a very early stage of the irradiation in both modelled alloys, whereas the quaternary alloys contain also Cu-containing clusters. Mn-Ni-rich clusters nucleate very early via a self-interstitial-driven mechanism, earlier than Cu-rich clusters; the latter, however, are likely to form via a vacancy-driven mechanism and grow in number much faster than the former. CRPs are, in essence, helped by the thermodynamic driving force to Cu precipitation in Fe, thereby becoming dominant in the low dose regime. The kinetics of the number density increase of the two populations is thus significantly different. These results are illustrated in Figure 11.

The main conclusion suggested by this task is that the so-called late blooming phases might as well be neither late, nor phases.

The above described results indicate that the atomistic modelling has provided an in-depth insight of the mechanisms responsible for the formation of nano-features in bcc-Fe based model alloys. These simulations are performed on relatively small boxes as they are very heavy to run even in the most recent computers. To allow for more flexibility and to consider bigger volumes that are representative of an RPV material, it is necessary to translate the gain knowledge into a more generalised mean field theory such as the kinetic rate theory.

In addition to the modelling effort, a substantial amount of experimental work has been carried out throughout the course of the project. It is worth citing two important achievements, namely, i)experimental examination of neutron irradiated model alloys and steels (issued from the PERFECT project left over materials) after post irradiation annealing, and ii) heavy ion irradiation, using JANNUS facility/France, to irradiate different model alloys in order to check the validity of the mechanisms described above. The results obtained confirmed the mechanisms described earlier in this section.

Another important source of information, that has been utilized by the project, concerning the formation of nano-features in RPV steels, has been the results obtained within the framework of the FP7-LONGLIFE, symbolized by a collaboration agreement that has been signed between both consortia. All the experimental data obtained from both projects are shared in the PERFORM 60-database hosted by HZDR in Germany.

The success indicators for this WP, established at the beginning of the project, are:

- Nanostructure evolution model for FeCuC alloys
- First approximation nanostructure evolution model for FeMnNi alloys

Both these indicators, have been achieved and the work has been extended to deal with an even more complicated model alloys such as FeNiMnSi(Cu), approaching closely the complex composition of an industrial RPV steel. In addition a substantial amount of experimental data adequate to validate these models has been made available.

I.2. Modelling of the flow properties of RPV steel

The main challenge of this task is acquiring and using the basic information which allows the computation of stresses and strains generated within an irradiated material under an applied external load. Knowledge of this behaviour is essential to simulate/predict the evolution of the mechanical properties and the brittle fracture of ferritic RPV steels.

For this purpose, constitutive laws are used in crystal plasticity to compute the macroscopic flow behaviour. To be accurate and reliable, these laws need to be physically founded. This means incorporating explicitly the mathematical description of the main mechanisms that are at the origin of the flow of the material, following the scheme depicted in Figure 12. The constitutive laws developed within the project, are able to take into account the major features of the plasticity of RPV steels: thermally activated slip, hardening mechanisms and dislocation interactions with irradiation-induced defects. These features are studied and quantified at the atomic scale by way of Molecular Dynamics (MD) using the interatomic potentials developed (see section. I.1), and at the mesoscopic scale by way of Dislocation Dynamics simulations (DD). The flexibility of the crystal plasticity constitutive equations allows the accurate description of the tensile curves for model alloys as well as for RPV steels (at least those identified as reference cases). An example of application to un-irradiated and irradiated RPV on the reference steel "EuroMaterial A" is given in Figure 13. It must be noted that, due to the homogenization method which computes the behaviour on a material point, it is not possible to predict the Lüder's plateau and the necking which are observed on test specimens. However, the effects of temperature and irradiation on the flow stress and the strain hardening are correctly predicted. Further, 3D aggregate meshes were used by finite element (FE) computations to determine the local mechanical fields. These local mechanical fields are implemented in the fracture toughness prediction model developed within the project (see chap I.3). A correct estimation of these fields needs a fairly good description of the morphology and of the crystallographic orientations. For this purpose, a library of realistic meshes of aggregates has been generated and integrated in the PERFORM 60 platform. In addition to the mesh library, software has been developed to obtain the FE meshes of the bainitic microstructure based on around 20 parent grains decomposed on 5-6 subgrains each (an example is shown in Figure 14).

The crystalline plasticity modelling has been applied on virtual bainitic aggregates obtained with the homogenisation method to compute the stress and strain fields in aggregates for morphologies and crystal orientations representative of the RPV steel. Different microstructures, triaxiality ratios and temperatures have been considered. The analysis of the resulting mechanical fields is performed on the maximum principal stress because this quantity is used in the brittle fracture modelling. A good agreement is found with numerical data in the uniaxial and triaxial cases and a slight shift is observed in the biaxial case (Figure 15).

The task has indeed been very successful, all success indicators promised at the beginning of the project, namely:

- Establish a roadmap with timescales to describe the improvement introduced in the computation of the macroscopic tensile curve in irradiated materials;
- Develop a new constitutive law to take into account the Carbon and irradiation effects;

have been reached.

In addition, a methodology to produce representative aggregates was also developed in this task. The resulting tensile curve is used both to evaluate the hardening due to irradiation and as an input to the fracture toughness prediction in the PERFORM 60 platform (see section I.4). Nevertheless, further developments are still necessary to improve the model, as for instance taking into account material heterogeneities at different scales and increasing the numerical efficiency of the developed codes.

I.3. *Modelling of the fracture behaviour of RPV steel.*

The main objective of this work has been to evolve existing models describing cleavage fracture in ferritic RPV steels based on micromechanical approaches. Firstly, special emphasis was put on the selection of suitable models and the identification of their potential for further development. Secondly, a selection of models for further improvement was made. In total four models with partly different scopes were selected. This combination of models had the advantage of covering a large field of application on the top end of the multi scale modeling chain treated in PERFORM 60 (as shown in figure 4):

a- A microstructurally-informed brittle fracture model (MIBF) based on crystal plasticity (described in section 1.3), which covers fracture prediction at the microstructural scale (sub-modelling) with possible extensions to include fracture prediction at the representative volume and specimen scales;

b- An advanced local approach model, based on the Beremin model, applicable to fracture prediction at the specimen scale;

c- The WST model which is foreseen as providing a link between sub-modelling and models of fracture behaviour at the representative volume and specimen scales;

d- A modified Bordet local approach model, which is regarded as an engineering model dealing primarily with the transferability of fracture toughness data from irradiated specimens to RPV ferritic steel components in service.

The selected models, their differences and specifications were clearly identified in order firstly to integrate them correctly in the simulation chain build in the PERFORM 60 computational platform and secondly to calibrate each of them using the same set of data called “reference data”. This work allows to be focused on the improvement of the physical understanding of the various model parameters and the origin of brittle fracture rather than to increase complexity of the model formulations themselves.

Based on the experimental data of these reference materials, specific reference cases were defined for each particular fracture model to calibrate its various parameters to verify its relevance to a specific industrial application. The prediction results were compared with experimental data to proof the suitability of the model.

For instance, the MIBF model (a) was calibrated on reference data then applied to other temperatures and fracture toughness specimen sizes. According to the calibration procedure pre-defined for this model, all parameters were considered temperature-independent (except stress-strain behaviour that is obtained from the work described in section I.2). MIBF simulations were then compared to experimental results. As example, Figure 16 shows the results obtained for 1T (C)T specimen. As it can be seen, except for the slope of the curve at T = -91°C, good agreement is obtained between simulation and experimental results for -154°C ≤ T ≤ -60°C and at the beginning of the curve for T = -40°C (before ductile propagation occurs).

As for the Beremin Model (b), the fracture toughness curve of irradiated material was predicted from the unirradiated data and yield stress change. The result is in good agreement with the irradiated data (Figure 17).

As for the WST model (c), 4 incarnations have improved significantly in terms of consistency via disassembling older approximations and introducing new features. The proposed and demonstrated calibration procedure has been shown to produce reasonable results applying a fairly compact and simplistic analysis procedure. WST predictions as compared to the classical master curve (Figure 18) for the constraint effect are quite promising and illustrate the exploitation potential of the model, and its micromechanical origins. The success indicators expected out of this task, namely:

- Selection and Integration of an advanced fracture toughness modelling scheme based at scale of sub-modelling and engineering models
- Establishment of reference cases to serve for the validation of the selected models

were partially achieved, as one of the models developed was not integrated in the platform and not all the reference data needed for the calibration of these models were available timely. Thus, further work is needed at least to benchmark all the existing models using the same set of experimental data and physically based calibration of the model parameters.

I.4. Integration of the developed models in the computational platform

The computational platform of PERFORM 60, was built on the basis of the one developed during the FP6-PERFECT project with the main objective to produce incremental versions. Four versions have been produced and distributed to the end users. The delivery was made in two formats: (i) a live–DVD, and (ii) an image file, which is available for downloading on the PERFORM 60 web site. The major improvement with respect to the former project can be summarized as follow:

<u>In the RPV module</u> :

- Improved parameterization for pure iron in the object kinetic Monte-Carlo (OKMC) including new models for migration energies, diffusion pre-factors, binding energies and defect traps, have been updated.
- A new rate-theory code "CRESCENDO" has been integrated. This code was co-developed to provide a stable numerical scheme and to overcome the limitation of the previous code "MFVISC2" by implementing several numerical optimizations, mainly, on what concerns multi-sink strengths and capture radii. Due to the assumption of homogenization needed to be considered in this type of codes, the parameters describing point defects and atomic diffusion and binding energies cannot be more than effective ones that have to be adjusted on the observed microstructure. Thus, these methods are quite robust in predicting the microstructural evolution in simple cases, but they need a substantial effort on the numerical parameterization of the physical data required. Nevertheless the RT implemented has been successfully validated by the End-user group, to check the effect of different irradiation parameters such us flux, temperature and irradiation dose.
- Update of the improved parameterization for low carbon iron in the object kinetic Monte-Carlo (OKMC) including new models for migration energies, rotation energies for 1D/3D motion, diffusion pre-factors, binding energies and defect traps.
- Rebuild of the RPV3 documentation based on a peer-reviewed article.

<u>In AFTM module</u> :

- A prototype of the large transformations for polycrystalline behaviour has been developed in Code_Aster. The associated validation and non regression tests have also been incorporated. This development was necessary to apply different modules for values of deformation beyond 10%.
- The Bordet model has been developed in Code_Aster and integrated in the platform. It is a post-processing model integrated in the fracture mechanic module. It is similar to the Beremin model (integrated in the platform during FP6-PERFECT), but it is supposed to better take into account the history of loading and the notion of active plasticity. The User documentation has also been supplied. A non regression test is also integrated.
- The new monocrystalline behaviour law (see section I.2) based on Dislocation Dynamics (DD) has been implemented in Code_Aster. It allows the behaviour of the vessel steel at high temperatures to be described. The development of DD_CC athermic in Code_Aster is a preliminary to the introduction of these new classes of crystalline behaviour laws issued from lower scales.
- The Finite Element calculations (in FlowBehaviour / Aggregate, FlowBehaviour/Homogenisation, FlowBehaviour/Correlation, FractureBehaviour /LocalApproach, FractureBehaviour/Correlation and FractureBehaviour /SubModelling sub-modules) have been updated with the last version of Code_Aster STA10.5.

- A new post-treatment has been developed to give the T0 parameter of the master curve approach from a single Beremin computation;
- Many improvements have been implemented as a result of the feedback from the User group in order to make the AFTM module more easy to use. In fact, the utilities have not always got all the required data to feed into the different sub-modules. Some evaluations procedures based on classical mechanical characterization are proposed.

I.5. SP1: conclusions and outlook

The progress made since the start of the project PERFORM 60 as compared to the former project PERFECT is summarised in a tabular form in Figure 19. Very impressive advance has been achieved concerning:

- Mechanisms of precipitation/segregation thanks to ab-initio simulations and the development of adequate and more sophisticated interatomic potentials such as: FeCuC, FeNiMn, FeNiMn(Cu),
- Interaction between irradiation induced defects and dislocations which leads to the development of a new crystal plasticity law based on dislocation dynamics
- Link between the microstructure and its changes and the evolution of the stress/strain field in RPV steels leading to a better prediction of the fracture thoughness using advanced models.
- Calibration and validated of the most advanced fracture toughness models on well controlled data set "Reference Cases"

Generally, PERFORM 60 has now build MSM tools to predict the « global » behavior of a generic « model » steels. The development of multi-scale/multi-physics models, as exemplified by the RPV tools, is necessary if accurate through-life toughness predictions are to be made: particularly in the context of extended NPP lifetimes to allow forewarning of possible adverse materials behaviour for flux/fluence conditions beyond current data.

Although, all success indicators have been reached and all deliverables have been achieved, the application of multi-scale modelling needs to be more focused on real issues such as:

- Understanding of the effect of metallurgical variables: local chemical composition (explain the role of chemical heterogeinities on the irradiation damage buil up).
- Evaluation of the effects of metallurgical heterogeneities and mechanical constraints on fracture toughness.
- Understand plasticity effect on fracture toughness
- Derivation of constitutive equations for irradiated material with explicit interaction between defects and dislocations as function of their type;
- Synergies between different phenomena in irradiated materials
- Uncertainty propagation analysis of the effect of the main parameters (T, dose, flux, chem. composition, …) on the rupture probability

It shall be noted finally, that the simulation platform developed for RPV steel within last decade shall be considered as an asset for the European community and shall be used further to get better feedback on possible improvement and simplification in order to make it useful for engineering applications.

II. Modelling of the initiation of irradiation assisted stress corrosion cracking on internals of pressurized water reactor: SP2

The modelling of irradiation assisted stress corrosion cracking (IASCC) involves the highest degree of complexity in the multiphysics chain, as it integrates aspects of radiation induced microstructure modifications, environmental interactions and mechanical behaviour, as illustrated in Figure 20.

The previous European integrated project, FP6 PERFECT, concentrated on the propagation of SCC. Within FP7 PERFORM 60, the major emphasis is on initiation of IASCC and its understanding and modelling. The shift from propagation to initiation is brought about by realizing that IASCC propagation rates could be relatively high and that a major part of the time-to-failure could be taken up by the period leading to initiation.

According to our present understanding, the time-to-initiation is made up by three periods; the precursor, the incubation and the slow growth period. The precursor is a period during which the material becomes susceptible to SCC in the specific environment and is associated with changes to the material and/or the environment. The incubation is a period during which marginal damage is regularly created (nucleation) but repeatedly repaired (healing). The slow growth period starts when additional damage is no longer sufficiently repaired, cumulative damage therefore becoming critical (embryo formation) a dominant crack forms and propagation takes over (Figure 21).

The introductory efforts made within FP6 PERFECT focused on the slow growth period and software to follow surface damage, INIT_EAC, was developed. In FP7 PERFORM 60, additional work in terms of the precursor and incubation periods was included, besides work to update the slow growth period. The work integrates irradiation induced microstructure modifications, environmental interactions and mechanical behaviour. Within project resource limits, and in accordance with the potential end-user interests, the work focuses on predicting IASCC crack initiation, with initiation in irradiated AISI-316 taken as the reference case. The project produced models at three different scales:

1. <u>Continuum scale</u>: A statistical model predicts distribution of cracks initiated as a function of time, load and material properties. The model is developed from the end product of the PERFECT project and represents a calculation framework for predicting the development of multiple cracks as a function of statistical and empirical rules. This scale relies on lower scale models for parameterisation beyond pure empirical data fitting. This modelling scale also provides the tool to compare experimental validation tests to the prediction.
2. <u>Aggregate scale</u>: At this scale deterministic models integrate mechanical and chemical contributions to crack nucleation and growth, and provide input to the statistical model at the component scale.
3. <u>Sub-grain scale</u>: This task provides mechanistic models combining the effects of oxide fracture, crack tip plasticity and grain boundary segregation.

The interdependency between the 3 different models is illustrated in Figure 22. It can be seen that the development of these models necessitates modelling tools to predict radiation-induced micro-structural changes and chemical segregation (section II.1), the degree of localized surface deformation (section II.2), the speed of re-passivation and associated material loss and the speed of oxidation along grain boundaries (section. II.3).

In these activities, the mechanisms contributing to IASCC initiation are identified from the characterisation of cracks observed either during the inspection of a nuclear power plant component, or from laboratory testing of well designed irradiated specimens. The relevant mechanisms are then translated into a mathematical form and the dominating material and environment parameters identified

II.1. Microstructural evolution and segregation induced by irradiation of stainless steel

The goal of this work is to produce the components of the INTERN end product for the prediction of the microstructure evolution of austenitic steels under irradiation, similar to RPV-module (see sections I.1 and I.4). This includes (i) prediction of the production of small scale (nm) primary damage and its evolution in terms of density, size and spatial distribution, (iii) prediction of the micro-chemical processes occurring under irradiation (e.g. radiation induced segregation (RIS)).

The work has been achieved according to the following steps (illustrated in Figure 23):

Step 1: Determination of the elementary properties and input for the RIS and microstructure modelling in terms of:

- Calculation of elementary data binding energies, migration energies and capture radii using ab-initio methods;
- Development of an interatomic potential (FeNiCr) that is used to mimic stainless steel;
- Determination of the fate of radiation damage (cascade debris) corresponding to different primary knock on atoms (PKA) to simulate a neutron flux.

Step 2: Development of micro-chemical and micro-structural models for irradiated materials for use in IASCC initiation and propagation modelling, by incorporating:

- For the microchemistry: a physical description of the microchemical processes occurring under irradiation, e.g. RIS at grain boundaries and precipitation, in model alloys for austenitic steels.
- For the microstructure: a physically based parameterisation and if needed modification of the existing mesoscopic models (MFRT and OKMC models) so as to be able to model the evolution of FeCrNi alloys (taken as “grey” alloys) under irradiation.

Step 3: Experimental validation of the micro-chemical and micro-structural models for irradiated materials of use in IASCC initiation and propagation modeling, based on:

- Experimental investigations performed on model alloys and reference materials.
- Transmission electron microscopy (TEM) study of the microstructure evolution in ion irradiated (without He implantation) stainless steels and model alloys;
- Tomographic atom probe (TAP), positron annihilation spectroscopy (PAS) and Field ion gun scanning transmission electron microscopy (FEGSTEM) analyses of radiation-induced microchemical changes in proton and ion irradiated austenitic model alloys (FeNiCr and FeNiCrSi) and model steels (SS 316) at several doses and different temperatures.

In order to quantify elementary interaction and mechanisms a large amount of ab initio calculations have been performed, in face centered cubic (fcc) Fe and in random (quasi random structure) Fe10Cr20Ni ternary alloys. The point defect vacancy and self interstitial formation energy have been calculated in both systems. In the fcc Fe system, for which calculations are easier, migration energies and the interaction of C and He have been quantified in addition.

At the atomistic level, a pair interaction model based on DFT calculations has been built and used to simulate thermal non equilibrium segregation (TNES) and RIS in a ternary FeNiCr alloy. A model for the grain boundary, which can be used also to model dislocations or loops has been developed. After some adjustment on the parameterization the Cr and Ni segregation obtained are in agreement with experimental results.

The main difficulties were the construction of atomistic cohesive models (mainly empirical FeNiCr potentials for microstructure and plasticity modelling) and the fabrication of the model alloys for the experimental part of this work.

In total, six embedded atomic model (EAM) potentials have been developed. One of them was found to be suitable for plasticity modelling with molecular dynamics. For the modelling of microstructure, it was found that none of the potentials are capable of describing correctly the expected stable phase for the ternary model alloy investigated in the experimental part of this project, due most probably to the complex magnetic characteristic of FeNiCr. To overcome this issue, a pair interaction model has been developed to model RIS by e.g. atomistic kinetic Monte Carlo (AKMC).

The microstructure has been modelled by rate theory and Monte Carlo methods such as the object kinetic Monte Carlo (OKMC). The parameterization has been improved to take into account density functional theory (DFT) data obtained within the project. A large effort has been made to develop, validate and qualify the rate theory code (CRESCENDO) (which has been rewritten based on the previous MFVISC code used in PERFECT). This allows performing robust simulation of the microstructure evolution.

At the macroscopic level, the RIS has been modelled by finite elements methods. Different models have been assessed and compared. The transport Onsager coefficient based on mean field theory (SCMF) have been used. The results are in agreement with experimental results, and in particular the solute profiles as a function of dose have been obtained, an example is reported in Figure 24.

Some additional work was dedicated at the atomistic or mesoscopic level to provide data, mechanisms or tools for the microstructure and RIS modelling:

- Displacement cascades have been calculated by molecular dynamics (MD), using the most pertinent FeNiCr EAM potential developed, as well as the binary collision approximation (BCA) cascades, to provide the source term for rate theory and OKMC.
- Relaxed Metropolis Monte Carlo has been used to assess the equilibrium microstructure predicted with the EAM potential developed.
- A mesoscale Cellular Kinetic Monte Carlo (CKMC) new method has been developed to model solute segregation kinetics similar to AKMC simulations but at a mesoscale.
- A phase field model has been adapted for irradiation modelling. It provides a mesoscale method taking into account explicitly a representative volume and elasticity.

It shall be emphasized that the last two mesoscale models (CKMC and phase field) are new original developments.

On the experimental side, a large matrix has been investigated under ion irradiation: 4 alloys, 2 temperatures (200 and 450°C), 3 doses (0.5, 1 and 5 dpa), 3 techniques (TEM, ATP, PAS). A very precise description of the microstructure has thus been obtained in terms of various features: segregation along dislocation lines and loops (Cottrell atmospheres), solute (Ni, Si and/or P) clusters and NiSi rich precipitates. In particular:

- ❖ TEM observations have shown the appearance of dislocation loops (Frank and perfect – the latest were not characterized), cavities and staking fault tetrahedral (example is shown in Figure 25).
- ❖ APT studies have shown the redistribution of Ni, Si and Cr under irradiation (Ni and/or Si Cottrell atmospheres and clusters, NiSi rich precipitates, Cr depletions associated to all these Ni and/or Si enrichments), an example of these characterizations is shown in Figure 26.

- ❖ PAS studies have revealed the presence of Fe single vacancies in the 316 stainless steel as the majority defect for high and low temperature irradiations, while in model FeNiCr alloy, irradiated at high temperature, vacancy clusters have been observed

The FEGSTEM study showed that radiation induced grain boundary segregation was exhibited by the binary Ni-Cr model alloy, in which the grain boundary had more Ni and less Cr than the general matrix. This suggests that the RIS was mainly controlled by vacancy diffusion. In more complicated alloys, despite the limited amount of specimens and as a consequence very small amount of grain boundaries suitable for careful GB RIS analyses there was generally a tendency to Cr depletion and Ni enrichment in vicinity of the grain boundaries, particularly as observed in all the obtained profiles from studied specimens of 316L stainless steel.

Furthermore, the stability of the microstructure has been evaluated by post irradiation annealing on the ion irradiated alloys, as well as on neutron irradiated commercial alloys**.** The experiments on ion irradiated model alloys showed that annealing seems to cause the formation of round objects that could be precipitates, possibly gamma prime precipitate, but this fact has to be confirmed in further experiments. Furthermore, indications of loop unfaulting were observed.

Finally, thermal annealing of neutron irradiated alloys indicate a reduction of the density of Frank loops and even their complete removal. A significant decrease of the void density was also noted at the highest temperature. These observations seem to indicate that the annealing temperature is a very important parameter, and that short post irradiation annealing experiments, combined with modeling is a suitable technique to distinguish the relative importance of microstructure features on IASCC.

As conclusion, it might be said that despite several difficulties in the modeling and experimental work, lots of progresses have been done in the understanding and modeling of austenitic industrial and model alloys under irradiation. The success indicators, expected from this task, namely:

- Production of FeNiCr interatomic potential based on thermodynamic and ab-intio data
- Improvement of the mesoscopic models to be able to predict the evolution of the microstructure and microchemistry such as RIS in stainless steels under irradiation

are unfortunately only partially fulfilled as the production of an adequate FeNiCr potential appears to be a very challenging task, and the mesoscopic models developed so far do not yet predict all nano-features observed experimentally. Thus, it is highly recommended to pursue this effort.

II.2. Modelling of irradiation induced hardening of stainless steel

This work focuses on providing both the tensile and creep behaviour of austenitic stainless under irradiation, with neutron-irradiated AISI 316 SS taken as the reference case.

In what follows, the main results of this work are given and clear indications on their limitations that require further work beyond PERFORM 60 are also included:

- ➢ Original and significant results about the interaction rules between dislocations and irradiation defects (mainly Frank loops) have been obtained for fcc structure based on the FeNiCr ternary potential and the results obtained are depicted in Figure 27, showing that Frank loops are the most resistant to the movement of screw dislocation at any investigated temperature provided that their size is larger than 4 to 5nm . However, decoration effects of Frank loops and mobile dislocations which are inferred from experimental investigations (APT and TEM as shown in Figures 25&26) were not investigated as the effect of Si need to be included in the simulations. More understanding of the role of decoration of loops by solute elements in the hardening process of irradiated stainless steels is strongly needed.

- DD simulations have clearly highlighted the role of small Frank loops (about 2-4nm) in the hardening process. Smart experiments are necessary to confirm this modelling output. Also the role of these small defects (the so-called black dotes) in the strain/stress localisation process needs to be further studied by DD simulations towards a full understanding of the deformation mechanisms of irradiated SS;
- A physically-based constitutive law for irradiated SS has been proposed at the grain scale. The superposition rule governing the hardening induced by different type of defects (FL, voids) has been taken as quadratic in this work. More extensive DD simulations would have been necessary to validate this latter hypothesis;
- Significant results have been obtained related to the description of clear bands, and the effect of their impingement at the grain boundary on the local mechanical fields. They demonstrated the rule of the clear bands in the initiation process and how their presence would affect the macroscopic behavior of an irradiated stainless steel. To complete this work, some verifications would have been useful such as i) the link between results obtained at the continuum scale (Crystal plasticity) and discrete scale (DD) ii) the role and nature of plasticity localization mechanisms involved in intergranular fracture of failed in-service bolts, although these observations are not available in open literature as yet.
- Effect of irradiation creep on the local and macroscopic mechanical fields has been evaluated based on phenomenological constitutive equations. The validation of this approach necessitates still some appropriate experiments such as in situ-TEM straining of irradiated stainless steels.
- Physically based constitutive equations at the grain scale have been developed and parameters determined from macroscopic experiments (tensile tests on polycristal). The obtained results can be considered are fairly good (Figure 28) when compared to the existing experiments.

The success expected out from this task, namely:

- Description of the hardening induced by dislocation-irradiation defect interaction as a function of dose based on mobility rules obtained from molecular dynamics simulations.
- Description of the local strain-stress fields at grain scale for irradiated austenitic stainless steel for different irradiation levels.

were partially achieved due, mainly, to the difficulty of developing an adequate interatomic potential, to simulate both the microstructural changes and the interaction dislocation-defects in the same time and also to the scariness of relevant experimental data in the open literature.

II.3. Modeling of the corrosion kinetics of stainless steel in PWR environment

The primary goal of this work was to develop and validate electrochemical models of the material-environment interface processes and their contribution to IASCC crack initiation. Since the structure and properties of oxides produced at the surface and preferentially at grain boundaries are viewed as key factors in the initiation of stress corrosion cracks, the aim of this WP was to characterize and model the oxide and its growth processes for irradiated 316L stainless steel and for a model alloy simulating the composition of grain boundaries suffering radiation-induced segregation. The work was broken down into three main tasks: i) experiments for model validation and calibration, ii) modelling of the oxidation processes, and iii) extending the corrosion processes to their impact on IASCC crack initiation. Due to the complexity of the processes involved, an important task in the first half of the project was the characterization of the corrosion processes and oxide product at the material-environment interface in both bulk and at grain boundaries in irradiated material, specifically:

- ❖ quantification of the main properties (composition, nature, structure, thickness) of the oxide film formed on a proton irradiated 316L exposed to nominal PWR primary coolant,
- ❖ determination of diffusion coefficients for oxygen in the oxide and influence of the irradiation (defects, strain localization) on these coefficients,
- ❖ collection of a database for modelling of oxidation.
- ❖ a parallel effort at computational modelling of the corrosion processes and resulting oxide character at the bulk and the grain boundaries was approached from several scales, including:
    - o development of Atomistic Kinetic Monte Carlo simulation of the oxidation of FeNiCr,
    - o extraction of oxide film properties from in-situ electrochemical and ex-situ surface analytical data for point-defect/mixed conduction model parameterization,
    - o point-defect/mixed conduction finite element model development for Fe-Cr-Ni alloy and grain boundary corrosion in B/Li solution under PWR-relevant conditions.

The calibration data for the models was generated using both an ion-irradiated 316 stainless steel and a high Ni and Si, low Cr model alloy simulating the composition of grain boundaries suffering radiation-induced segregation (GB-RIS). Autoclave tests by all the partners were carried out in PWR conditions. Brief autoclave exposures carried out by EDF on GB-RIS materials indicated a slightly lower oxidation rate for this material. Oxygen tracer experiments confirmed a measurable influence of irradiation on O diffusion, with the diffusion rate being faster in oxide formed on the non-irradiated sample. In long term autoclave exposures, the effect of exposures at only 200ºC was a thicker oxide at lower pH than at higher pH, which is the reverse of what was observed at 325ºC.

Results for 316L and GB-RIS model alloy specimens exposed to PWR conditions for 2 minutes already showed higher Ni and lower Cr in the inner oxide layer on the GB-RIS model alloy, which was also thinner than on the 316L. Ni was enriched and Cr depleted at the substrate interface in both cases. Additional experiments specifically targeting transport properties, namely the oxygen tracer experiments, and the transport property extraction from oxide composition profiles, were reported along with the respective transport property extraction results.

Long-term exposures to variations of PWR chemistry was apparently more sensitive to the particular conditions than to whether or not the material was proton irradiated or cold worked (Figure 29)

The above described experimental data were used to calibrate a model of oxidation rate of non-irradiated 316 SS in PWR conditions at normal pH 7 and elevated pH of 9.1 (where oxidation was more rapid), at both 200 and 325°C (as shown in Figure 30). Detailed analyses were also conducted in order to evaluate the effect of strain on oxide penetration, based on EFTEM Cr-map analysis. Results suggested an increase of the mean oxide penetration with the local cumulated axial deformation. At the meso-scale, the original parameterization of the mixed conduction model was carried out based on EIS measurements. XPS data from exposure experiments were then used to update the parameterization. New transfer function derivation addressed open questions related to the form of the impedance of transport of ionic defects. A main challenge tackled was the boundary conditions at the alloy/inner layer interface.

With regards to linking meso-scale process models with finite element modelling, a new model, called the SF-PDM (Spinel, Field-Point Defect Model), was developed. The model explicitly takes into account the alloy's elements in the film - there have been very few attempts made in the literature to do this, most treating a film containing one metallic constituent only. The model takes the substrate composition into account, and expands it to two dimensions. Since the interfacial rate constants and diffusion coefficients depend on the local concentrations of species within the film, the model can be used on Fe-Cr-Ni alloys of varying composition without changing the parameterization. With a view to assess the effect of vacancy injection on IASCC crack initiation, a detailed literature review has been carried out to compare oxide formation in plant failures versus laboratory tests, suggesting that there may be a difference. Fracture surface oxides formed on stainless steels during in plant exposure and during laboratory testing in simulated environment are very similar. The crack advance in irradiated material can include environmental contribution due to oxidation. Oxidation, especially, duplex film formation on fracture surfaces includes diffusion of atoms from the bulk metal to the oxide, leaving vacancies in the bulk metal near the crack tip. Corrosion-induced vacancies may contribute to the initiation of stress corrosion cracks through the so-called selective dissolution, vacancy creep model.

Progress in the Atomic Kinetic Monte Carlo approach to modelling the growth of the inner layer oxide has benefitted from receiving the ternary potential developed in the project. The approach to achieve the development of AKMC simulation of the oxidation of FeNiCr was the extension of a Virtual Oxide Layer (VOL) model for layer growth on binary alloys to the simulation of ternary alloys and the calculation of certain parameters determined empirically in the pre-existing VOL. The main improvement of the VOL model over the previous model is the fact that it is truly 3D – solid state diffusion in the bulk of the alloy and the oxide contributes to the growth of the oxide layer, in addition to the surface processes which have been considered the sole contributors in the former model. Furthermore, instead of using Metropolis Monte Carlo, the Kinetic Monte Carlo (KMC) algorithm was employed; Figure 31 is a schematic description of this model.

The expected success indicators out of this task, namely:

- Modelling of the oxidation kinetics taking into account the composition of the matrix when exposed to nominal PWR primary water,
- Parameterisation of irradiation creep enhanced corrosion model for stainless steels in PWR conditions,

were reached, in addition an important amount of experimental data have been generated both on the corrosion kinetics and the microstructure of the oxide films that would certainly help generating more robust models.

As stated earlier, all the work presented in sections II-1 to II.3 has been used to develop two important codes that integrate most of the information listed above. In the following, a short description of each of them will be given before demonstrating their ability to predict the initiation of IASCC phenomenon in PWR internals.

II. 4. Statistical model for the prediction of IASCC initiation: INITEAC

Within the framework of the PERFORM 60 project, the statistical code INITEAC has been developed to simulate crack nucleation and growth with the aim of predicting crack length distributions obtained from multiple runs of the program. Originally a code-generated pattern of hexagonal grains was used to provide the boundaries the cracks grow along. In a first upgrade this has been extended to arbitrary grain boundary patterns provided by the user to the program. In addition, a general sensitivity formula has been implemented that enables several parameters influencing SCC susceptibility to be defined for each boundary. Comparing INITEAC with experiments on model alloys (unirradiated) the following conclusions were drawn:

- INITEAC was found able to reproduce main trends in the experimental data from tests using non-irradiated model alloys. Fitting the input parameter to data from one material INITEAC correctly predicts trends in the measurements on a different material. Experimental data with very few cracks per area could only be reproduced very roughly due to poor statistics in the INITEAC results. This could be improved in the future by increasing the statistical variability of results from INITEAC runs with the same input parameters.

When using INITEAC to simulate irradiated specimen tests:

- By adjusting three input parameters of INITEAC whilst using best estimate values for all other input parameters it has been possible to reproduce the major features of the experimentally observed threshold curve for irradiation dependent failure, as illustrated in Figure 32. Indeed, the results obtained are in fairly good agreement with the experimentally driven curves which indicate that the ratio between the applied stress and the yield stress of the material would decrease by increasing the neutron dose (operation time).Shortage as well as scatter of experimental data for the dose dependence of yield stress, Si and Cr concentration gives rise to large uncertainties in the results from INITEAC.

Future steps in order to improve on this uncertainty should therefore include the acquisition of more experimental data and the improvement of data quality. Beside this, additional effects (such as Ni segregation) could also be considered to be included in INITEAC.

II.5. Deterministic model for the prediction of IASCC initiation: IGOC.

The Intergranular Oxidation and Cracking (IGOC) sub-module describes the true initiation and the following successive crack extensions due to IASCC at the scale of the polycristal. The assumed mechanism is based on the oxide penetration on grain boundaries and the following evaluation of the resistance to fracture of the grain boundary affected by the oxidation, considering the oxide itself and the local modification of the chemical composition of the metal, at the grain boundary, ahead of the oxide. The scheme used to gather all the necessary ingredients to develop this end product is illustrated in Figure 33. The actual approach is deterministic. The typical **scales** of the model are:

- 10^{-2} mm^3 (équivalent to about 200 grain-polycrystalline aggregate).
- 1000 h (duration of SCC test in the laboratory).

Voronoi space subdivision is used to model polycrystalline aggregates. Oxidation kinetics was provided by the work described in the section II.3. Crystal plasticity modelling is an appropriate approach to evaluate the heterogeneity of the continuous mechanical response in an aggregate, taking into account activation of slip systems. Therefore, such modelling is relevant to simulate IGSCC mechanisms, where hardening and stress concentration at grain boundaries play a significant role in the cracking mechanism. In the final version of the platform, the phenomenological behaviour has been replaced by the crystalline plasticity law indicated in Section II. 2, in order to incorporate the physics and the irradiation effects. To model the initiation and the extension of the crack along the grain boundaries, cohesive elements are inserted between grains. The crack propagates using Cohesive Zone Model (CZM) laws whereby crack opening costs energy proportional to the crack length. Specific routines were developed in Python language and introduced in a Code_Aster computation to simulate the IGSCC due to local coupling between mechanical parameters, oxidation and fracture. Grain boundaries are weakened by oxidation as soon as the Gauss points of a CZM are reached by oxidation. Therefore, crack extension depends on two parameters: the local intergranular oxide penetration and the local stress applied on the grain boundary weakened by oxidation. An example of the results that could thus be obtained is depicted in Figure 34, showing as expected that highly irradiated materials are more susceptible to IASCC. Further work is needed to increment the robustness of the approach, to increase the efficiency of the platform and to implement more physics in the parameterization of different models.

II. 6. SP2: Conclusions and outlook

Multiscale modelling addressing many of the issues for prediction of IASCC has been an important part of the PERFORM 60 project. Particular successes and remaining limitations that are worthy of further study beyond PERFORM 60 include:

- Modelling
  - The framework document created early in PERFORM 60 remains a valuable reference for modelling experience and mechanistic insight. It has guided a significant amount of the PERFORM 60 modelling, especially at the continuum scale.
  - There has been significant progress modelling the effects of localised deformation in terms of grain boundary stress concentrations arising from clear bands, and grain boundary stress/strain fields due to irradiation hardening . However, work is still needed to guide on conditions leading to localised deformation.
  - There has been incorporation of the effects of localised deformation into the continuum scale INITEAC IASCC model, whereby equations defining GB increased susceptibility due to localisation are used. Presently these rules are not able to be used until further parameterisation has been possible.
  - Modelling of surface oxidation in PWR primary water, including sensitivity to matrix chromium composition, irradiation creep, localised deformation and environment. These models have been developed and validated using experimental data. Development of the models to predict intergranular oxidation would be useful.
  - The oxidation rules have been incorporated into the continuum scale models IGOC and INITEAC Ability to adjust sensitivity of oxidation rules to chemical compositional variability is presently only for chromium content. It would be useful to be able to model other effects of Radiation Induced Segregation.
  - It has been possible to reproduce to reasonable accuracy the current accepted variation of the ratio between applied stress and the yield stress of irradiated material versus dose, predicting therefore the IASCC threshold using INITEAC. With greater quantities of experimental data on IASCC initiation,, it would be possible to use this model to explore sensitivities to irradiation conditions etc, to the benefit of IASCC understanding.
  - The synergies between the deterministic IGOC model and the statistical INITEAC model have been demonstrated whereby parameterisation can be done in IGOC and the results then used in INITEAC.
- Experimental data
  - Some limited empirical data has revealed oxide fracture conditions for proton irradiated 316 SS; it has also been interesting to see an apparent correlation between dislocation channelling and rupture of surface oxides. However, no rules able to be used in continuum scale models are yet available, neither does the data extend above low dose.

- Qualitatively, a dependence of strain localisation on dose has been seen, it also seems that loading conditions affect the degree of strain localisation. More well designed lab. experimental data would be needed to develop quantitative rules on localisation able to be adopted in IASCC models, even though the final validation should take into account the failure modes observed in real operating conditions.

To sum up, the table of Figure 35, illustrates the progress made within the PERFORM 60 project taking as starting point the situation at the end of PERFECT project.

III. Sub-Project 3 "Users' Group"

The scientific approaches developed in the SP-1 and SP-2 sub-projects to model the behaviour and degradation mechanisms of reactor pressure vessel (irradiation embrittlement) and internals (IASCC) materials are very innovative both because of the techniques used for numerical simulation and of the challenge to derive the macroscopic component behaviour from the microscopic evolutions of the material.

Although this project deals with fundamental research and modelling, it's a challenge from an industrial point of view, since only such an in-deep physical understanding of the degradation mechanisms is able to provide predictive modelling of these phenomena.

Therefore, to fully reach the goals of the project, a complementary work has been done through a Users' Group in order to assess the developed modelling with industrial data and share the knowledge and modelling approach improvements among the European and International nuclear Communities. The work included, first of all, the establishment of a consensual view through the compilation of the state of art knowledge with a critical evaluation of existing tools and approaches in a 60 years operation context. Secondly, a large collection of experimental reference data and proposals for industrial applications. Finally a trough out evaluation of simulation tools has been performed to address their applications to collected reference data and applications.

Taking into account the lessons learnt from the PERFECT Users' Group, The activity of Users Group has started at the beginning of the project in order to constitute a wide diversified UG. In fact, a wide participation has been noticed, including various organizations from Europe, USA and Japan representing utilities, R&D organisations, manufacturers, regulatory and safety organisations. A working programme has been defined for each organisation using a specific "participation agreement" that has been signed by the coordinator on behalf of the consortium and the interested organization.

The activity of the Users' Group SP-3 was split into 4 major tasks:

- Constitution of Users Group (involving external partners of the project with a specific contracting to set up), including its management and coordination, reporting and feedback towards other members of the project (SP-1 and SP-2), organization of specific Training sessions on simulation tools, and the external communication.
- Scientific and industrial evaluation of the simulation tools and their capability to be used in the future for practical industrial applications and assessments (and how to fill the possible remaining gaps).
- Collection of reference data and industrial applications, both for RPV and Internals materials. All these elements have been gathered in a specific database (PERFORM 60 Database) using feedback from previous FP6-integrated project PERFECT. This work included the constitution of the Database, the definition of input and output data, the Quality Assurance of the Database, and its maintenance which is of special interest for industrial applications related to:
    - Materials: chemical composition and manufacturing;
    - Specimens including cutting schemes;
    - Irradiation conditions;
    - Metallographic and microstructural investigations;
    - Mechanical test results and fracture mechanics testing;

- Atomistic modeling.

A wide range of materials has been inserted in the database, notably including:

- Western RPV steels;
- Western weld metals;
- VVER type base metals;
- VVER type weld metals;
- Laboratory materials

Notice that there is no model alloy in the database.

- A final evaluation of simulation tools and end products and their ability to be used in real industrial components assessment.

To achieve the above tasks, it was necessary to organise two dedicated training sessions. The first one has been organised from 15 to18 March 2011 at EDF-Les Renardières, in which more than 50 participants out of 32 organisations have attended. The scientific and technical progress of SP1 and SP2 has been widely presented to the Users Group addressing the capabilities and limits of the models and the tools, including first demonstrations of the PERFORM 60 platform (V1.0). An updating of UG work programme has been discussed with all participants. The following contributors were then committed to be active in the user goup: HSE-NNL/UK, (including financial support to NNL for further examination of the microstructures), EDF (some more data out of its surveillance programme with additional characterization, Rolls Royce, IRSN (as user of the platform), AB Ringhals / Vattenfall (to provide private data), Tractebel Engineering (to provide private data), AEKI / KFKI, TEPCO, ORNL (comparison with DISFRAC), EPRI (Evaluation of the tools on both RPV and internals), AREVA GmbH, NRI, BZF (coordinates a common contribution on VVER steels with NRI & Prometey), KAERI. Other organisations have engaged in addition their in-kind contribution and become very active inside the project, such as PROMETHEY/Russia, CNEA/Argentina, Uni-Helsinki/Finnland, NNL/UK, CRIEPI/Japan.

Based on this first group who signed the participation agreement, the 2nd training session has been organized again at EDF Les Renardières on 15-19 April 2013, with a wide participation (57 registrations from 21 organizations) with the main objectives of:

- Informing participants about final progress of the PERFORM 60 project;
- Presenting and demonstrating the project database;
- Giving the status of developments and corresponding description, elements of validation (models and tools).

Right after this training session, the evaluation of the version 3.0 of the platform has been made leading to the following results.

a- Evaluation of the PERFORM 60 platform for RPV

The initial evaluations were done by UG members through Apollo-database that was installed in the Huddle workspace of the project website. There followed a Joint Evaluation Meeting (Paris, 1-3 October 2013), in which additional evaluations were done. The Live DVD has 15 modules that produce an output that can be compared with available data, scores of alternative chains of modules leading to a prediction of the same observation, and around 130 model parameters. It was not feasible to investigate more than a small fraction of the potential alternatives within the resources available. Nevertheless, it was possible to achieve a reasonable depth of coverage encompassing most modules. The original target for the total number of evaluation objectives was exceeded and the number of prediction results was substantially beyond expectation.

Given the limitations of current knowledge and computational techniques, the RPV tool evaluation generally performed fairly well, and demonstrated potential for future practical application. Some modules could not, however, be fully tested due to limitations of the implementation of the models on the Live DVD or lack of suitable comparative experimental data. It is clear however, that there are still significant limitations in current knowledge, and that it is difficult to make full extent of the modelling advances available using a Live DVD format. But, even with these limitations, the RPV tools are already valuable for training and development of insights.

The scientific and technical level of tools was underlined during the final workshop, but the platform and the simulation tools seem to be more appropriate for developers and model experts (‘academic tool’) than for common users in link with real industrial applications.

b- Evaluation of the PERFORM 60 platform for internals

Most of the validation exercise was concentrated on the one hand on the microstructure tools and, on the other hand on the INITEAC software, which is not integrated on the Live DVD but was provided as a stand-alone version. The available tools can at best reproduce the general trends seen in the field, which is interesting for academic or training purposes, but are still far of having reliable predictive capabilities. In addition, they require a specific expertise in and knowledge of the physics and models for each of the modules which most of the time is not available for the average end-user.

The target audience of multi-scale, multi-physics models in the field of IASCC should rather be the scientific community active in this field in laboratories and research institutes, and not industrial end-users who need robust and relatively simple engineering-type models in order to provide the data necessary for structural integrity assessment or lifetime prediction of plant structures and components. The multi-scale, multi-physics modeling could help developing such models on the basis of physically sound principles.

It was acknowledged that the tools developed in the project represent a remarkable achievement from a scientific point of view, but the live DVD cannot reflect the full extent of the work. Many of the modules developed for the Internals are not fully implemented on the Live DVD and could not be tested by the Users’ Group. Some modules provide intermediate information which is probably useful to help researchers understand the IASCC mechanisms or to test specific hypotheses. However, it is of limited usefulness for the industrial user, which does not have the necessary data or the expertise to run these tools and is not necessarily in a position to appreciate the scientific value of the work. The final result is still of limited practical use for the lifetime management of the internal structures of an operating reactor.

Potential Impact

The impact of PERFORM 60 is rather of strategic nature, as it allowed strengthening the ***leading position of the EU's nuclear industry*** in the field of numerical simulation for residual lifetime prediction. It is in fact effective to date, PERFORM 60 developed tools are , to a certain extent, able to predict radiation effects both on RPV steel's (bcc crystalline structure) mechanical behaviour and initiation of failure of austenitic stainless steels (fcc crystalline structure); Thus, the PERFORM 60 project allowed the community settled, already within the FP6-PERFECT project, to take a dominant position in the frame of fracture mechanics and stress corrosion cracking simulation fields. Furthermore, the results obtained are very encouraging to become directly applicable to existing reactors up to possible 60 years of operation. Moreover, the studies conducted within the PERFORM 60 project are considered to be of great interest for GenIV reactors. Indeed, even if the materials involved in GenIV reactors are different, the numerical tools developed in the frame of PERFECT and PERFORM 60 are able to take into account 2 types of crystalline structure, i.e. bcc and fcc. No doubt that these kinds of crystalline structure will be present in GenIV reactors. One can also list several other potential impacts that are addressed by the PERFORM 60 project, such as:

Capitalization of knowledge: During the last decade and thanks to both projects (FP6-PERFECT and FP7-PERFORM 60), a huge effort has been dedicated to capitalize the experimental and theoretical works that were carried out to characterize, understand and model irradiation effects in materials since the sixties to the eighties, both by integrating and developing new simulations tools based on this knowledge and also by creating a dedicated database storing the most relevant data set to validate the models at the appropriate scale. Thus, the future European Research in these fields can benefit from the amount of work performed twenty to fifty years ago.

Structuring of the European Research: PERFORM 60 brought together around 20 research centres, institutes and academic laboratories working in the field of numerical simulation of materials behaviour. In addition, close collaborations have been settled with the main players in the field worldwide (see User's Group) such as the programme CASL in the USA, the programme PLIM in Japan and those under investigation in Russia and Korea. Such a large international community is indeed required to mobilize the necessary competences and skills; no single country could provide all of them.

Training: Learning about irradiation damage requires a strong involvement of students from academia and young engineers from industry. Indeed, the tools developed allow to carry out “virtuel” experiments aiming at assessing systematically the cross-influence of parameters (temperature, spectrum,…). The simulation tools developed are now being used in many training activities across Europe and even the world, just to quote a few of them:

- European master in nuclear engineering hosted by Paris-TECH/France;
- Master of nuclear engineering at the institute of nuclear technology and science (INSTN/France);
- The yearly training courses for young engineers organized by the Materials Ageing Institute having as constitutive members the most important nuclear energy producers in the world namely, EDF SA (FR), EPRI (USA), KANSAI/INSS (J), EDF-Energy (UK), CGN/SNPI (CN), Rosenergoatom (RU);
- Formation of young engineers at SUEZ/Eletrabel;
- Course on nuclear engineering and materials by ENEN.

In addition, the project itself contributed to many topical schools and organized two specific ones and it is listed later.

Bridging "Eastern" and "Western" countries: The PERFORM 60 project played an important role in the dissemination of recently developed codes and knowledge concerning numerical simulation of materials(see later the composition of the user group). This dissemination was particularly fruitful within Eastern countries as many seminars have been provided in the interested research institutes or academia by PERFORM 60 contributors.

Disseminating European Research among non European countries: The fact that the user group, has members from all over the world including EPRI/USA, PROMETHEY/Russia, KAERI/KOREA and TEPCO, CRIEPI/JAPAN ensures that the results provided by the European research have been disseminated among non European countries in addition to more than hundred of international peer reviewed publications and key notes oral presentations.

a- Socioeconomic impact

The socio-economic impact of the project is realized through:

- Enhancing industry innovation: the tools developed within the project will allow a better use of resources concerning the assessment of the reliability of the main structural components of nuclear power plants. They are certainly helpful in planning adequate surveillance and maintenance programs for the RPV and its internals. They will also provide a technical basis envisaging innovative solutions on in-service repair and or mitigation of radiation damage of these two critical components, namely the RPV and its internals.
- Creating growth by enhancing the availability of nuclear power as it can help reducing the maintenance and inspection durations of the two studied components (RPV and internals). The lifetime of a nuclear power plant is technically related to the integrity of the pressure vessel among others. To ensure a smooth energetic transition in Europe, and to allow for a safer operation of the existing NPPs, it is of paramount importance to be able to assess the residual lifetime of the critical components such as the RPV.
- Enabling small and medium size enterprises to benefit from improved model tools as in the course of the project few SME's have interacted with the project consortium either to provide advanced IT services (i.e. Phimeca/France, LGI/France, EMDESK/Germany).

b- Societal implication of the project

More than 330 persons have contributed to the success of this project. About 280 persons have contributed to the scientific achievement while 50 members, have used actively the results and trained with the developed software platform, as end users.

Among the scientific and technical contributors, more than 150 are experienced researchers (40% are women), about 90 highly qualified personnel (35% are women) and about 30 young engineers, post-docs, or PhD students (15% women). About 10 new jobs have been created within the consortium.

This high qualified community has first of all learned to work together in spite of cultural and organisational differences and they were able to collaborate together towards commonly decided objectives within the project.

Indeed, as it is demonstrated in the following sections, the project appears to be quite attractive to create renewed interest to the nuclear engineering, material science for nuclear application as the approach developed is very challenging and considers the latest development in new technologies: namely computer science and communication.

Use and dissemination of Foreground

Within the project, 2 summer schools and two international workshops have been organised

1. **MATRE-1 summer school**

The First International School on Materials for Nuclear Reactors (MATRE-1) was jointly organised by FP7/GETMAT and FP7/PERFORM 60 projects. It was the first school organised in the framework of both projects. It was held on the premises of the Auberge de la Ferme in Rochehaut sur Semois, on the Belgian Ardennes, from 18 to 23 October, 2009. 45 'students' ranging from undergraduate students to senior scientists, but mainly PhD students participated in the school: 29 men and 16 women. They were sent by laboratories located in 12 different countries and represented 15 nationalities. Sending laboratories ranged from universities to research centres, industries and also safety authorities. The technical programme included both lectures and interactive sessions. In addition, a poster session was held to allow students wishing to do so to present their research work. 24 posters were presented and the three best posters, as voted by students and lecturers, were awarded a prize.

2. **SOTERIA summer school**

SOTERIA[2] is the international training symposium on irradiation effects in structural materials for nuclear reactors, jointly organised within the framework of two FP7 collaborative projects, namely LONGLIFE and PERFORM 60. It was held in Seville, Spain, from September 17 to 21, 2012. The main aim of the symposium was to train early career researchers and senior engineers on topics of relevance for both the operation of existing nuclear power plants and for the implementation of the next generation reactors.

The University of Seville freely offered its facilities for the symposium, specifically at the School of Architecture. The training programme covered five days, equally distributed among two sections: RPV and internals. The interactive sessions were based on the use of the tools developed in PERFORM 60 for the simulation and prediction of radiation effects in steels. These tools have a potentially high educational added value, as they allow a student, under proper guidance, to perform virtual irradiations, with the possibility of "seeing", as if using a sort of virtual microscope, the nanostructural changes produced in the material, observing how they evolve with dose and checking the effect of variables such as dose-rate and temperature. Next, the student is given the possibility of simulating the effect of these nanostructural changes on the mechanical properties, in terms of increase of yield strength and reduction of ductility. These are the effects of importance for RPV steels. On the side of internals, similar tools have been developed but, in addition, the possibility exists of looking at the development of irradiation assisted stress corrosion cracking, which affects specifically austenitic steels.

In parallel with the symposium, a workshop on "hot issues" in radiation embrittlement was held on the first day, open to experts present at the workshop.

In total, 122 delegates participated in the symposium, including organisers, lecturers and students. 29 lectures and 2 interactive sessions were given to 83 students by 32 lecturers. Women represented about ¼ of the participants. While most students were in their early career, many 'advanced' students also attended. The participants came from 48 different organisations, distributed in 17 different countries. About 80% of the organisations represented at the symposium were European, but there was also an important presence from the USA and Russia. The organisations were equally

[2] Soteria was the Greek goddess of Safety

subdivided in ~50% research and ~50% industry, even though the latter often corresponded to R&D divisions (e.g. EDF R&D).

3. PAMELA international workshop

The workshop PAMELA, dealing with "*Predictability of long-term ageing mechanisms of reactor components based on modelling and laboratory experiments*; has been held at Mol/Belgium from Sept'19 to 22d, 2011, with the aim to address the issue of the transferability of data - from accelerated experiments performed in the laboratory, to the conditions met by the material when in operation - based on advances in modelling and on a proper analysis and correlation of existing data, from both laboratory experiments and surveillance. 75 participants out of 30 organisations from 16 countries (utilities, producers, research centres and universities,…) have attended the workshop. About 25 invited talks and 45 posters have been presented and discussed.

4. Final workshop:

The International workshop on "multiscale simulation of the prediction of radiation damage in reactor pressure vessel steel and internals up to 60 years of operation" was held at EDF-Les Renardières, Moret sur Loing/France, from 10/12/2013 to 12/12/2013.

The main aim was to demonstrate that the commonly deployed effort, that is to develop future tools useful for industrial and research projects, related to the prediction of materials behaviour under nuclear power plant operating conditions, has been widely disseminated with the scope to provide:

- A sharp **understanding** of the physical phenomena and interaction between them (experimental tests, observations).
- An **accurate definition** of the several blocks needed for the modelling (problem splitting into sub- domains in time and space) **– ˝localisation strategy˝.**
- The **simulation** (as accurate as possible) of the observed local phenomena and interaction between them.
- The use of powerful numerical tools to homogenize in time and space – **˝homogenization strategy˝.**
- The **validation** of the tools using representative in-pile experiments.

This workshop had therefore the objective to bring together all the contributors (developers, users, ...) to this project to share their knowledge and to present the main achievements obtained within the project as part of its dissemination strategy. Furthermore, the workshop is open to the whole international community.

The workshop hosted 110 delegates coming from 23 organisations from all over the world, including USA, Russia, Korea, Japan and Europe. The workshop started with 3 invited talks: from USA to describe the scope of the CASL project sponsored by the DOE, Japan to present the actual national programme regarding the modelling of material behaviour and finally from Russia to report on the main outcome of the ISTC # 3973 project on residual life assessment coordinated by PROMOTHEY institute.

The workshop was also the occasion to present and discuss the review and evaluation of both the most important deliverables by the evaluation and review committee that has been appointed by the project executive committee and the tools integrated in the simulation platform by the user group as will be described in some details in the next paragraphs.

Other Communication/dissemination events

All the members of the consortium have been active in disseminating the results. More than 60 articles have been already published in international journals with peer reviews, the same amount have also been reported in proceedings and more than 50 invited lectures have been given at many occasion. In addition, the results and especially the simulation platform is being used continuously by many organizations in their daily practices.

Here it is worth mentioning that the technical representative of the coordinator has presented the project is several European and international events. Indeed, the project has been presented at the following events: NULIFE and NUGENIA Fora, IGRDM15, IGRDM17, SMIRT22, CORROSION 2013 where a special session was dedicated to present and discuss the content of the SP1 project. The project was also presented at the ICG-EAC-2010-2011-2012-2013, at international conferences such as MMM-2010 and 2014, ICACM2010 and Fontevraud 2010 and 2014, GORDON, MRS and many others. It was also presented at the FISA 2009 and FISA 2013 conferences organized by the European Commission. The project has been under the umbrella of NUGENIA and part of its portfolio since 2011. A state of the art document is planned to be published under the NUGENIA label.

Scientific and technical evaluation and review committee

To assess and ensure the high quality level of the scientific production from PERFORM 60, it was decided to organise the « Evaluation and Review Committee» (E&RC), that was composed of 6 prominent scientists in the fields of material sciences, mechanics, corrosion, solid state physics and irradiation damage. The ERC had the following main objectives: a) to assess the scientific research output, b) to make recommendations to Sub-Project Leaders (SPL), c) to propose possible scientific improvements and/or reorientations to SPL, d) to support the coordinator for EC evaluations. The ERC members were:

- ✓ Chair: Damien FERON, CEA, (Corrosion)
- ✓ Colin ENGLISH, Oxford University, (Microstructure and fracture aspects, IASCC).
- ✓ Jean-Louis BOUTARD, EFDA (retired in 2009), now expert attached to the CEA (Atomistic modelling of radiation damage)
- ✓ Sylvain LECLERCQ, EDF, (Flow behaviour /creep under irradiation)
- ✓ Marc HOU, University of Brussels (ULB), (Microstructural evolution/segregation)
- ✓ Dolores GOMEZ BRICENO, CIEMAT, (Corrosion behaviour, SCC)
- ✓ Ulla EHRNSTEN, VTT, (Corrosion behaviour, IASCC)

This committee had as a rule to critically review all the reports issued by the partners, and organized several face to face meetings with the project executive board.

E&RC Review of the scientific and technical achievements of PERFORM60 project

The members of the ERC have greatly appreciated the description of the project status and the overview of the main achievements and issues given by the PERFORM 60 coordinator and the SP leaders (during the 3 dedicated meetings). The ERC dealt mainly with the SP1 and SP2 scientific outputs and its members appreciated very much to have information on the SP3 developments.

For RPV: an important concern is the fracture toughness. To cover different scale lengths, several models have been identified for further developments and integration in the PERFORM 60 platform. They were selected with the aim at incorporating lower scale modelling into the upper scale, to link the local approach to the engineering models. Materials (RPV base metals, welds and model alloys) with which to validate / verify the various models of flow and fracture behaviour being developed in SP1 have been selected jointly with the FP7-LONGLIFE project and form the basis of reference cases.

A substantial effort has been undertaken to develop new methodologies to derive interatomic potentials for FeCuC and FeNiMn based on the ab-initio and thermodynamics calculations performed. The FeCuC potential, used to mimic the behaviour of high Cu RPV steel has been fully exploited to derive the interaction rules between irradiation induced defects and dislocations leading to the necessary parameters for the meso-scale modelling of either the microstructure or the dislocation dynamics. As for the FeNiMn potential, the task appears to be much more difficult than expected but still a first version of this potential has been made available and will have to be tested further against the experimental observations, to ensure its robustness.

Regarding Internals, the main concern is the comprehension of the individual mechanisms contributing to IASCC and the interactions between irradiation, corrosion and mechanical loads. In particular, the main goal is to identify the most important features participating to the crack initiation. The role of corrosion has to be better understood as well as the radiation induced segregation and the contribution of local strain gradient.

Efforts are made on crack initiation criteria for which modelling results and experimental data are compared. Analytical models of crack initiation are based on a strong interaction between dislocation channels and grain boundaries, using an energy balance criterion. Results are in agreement with experiments performed with slow strain rate tests (SSRT) in inert environment. However, on irradiated specimens, no clear bands are observed in the SSRT under PWR environment. A statistical tool (INITEAC) is also developed with success to predict reasonable maximum crack depths and also the numbers of cracks, based on criteria which indicate the failure and are tuned to obtain the best comparison. Being able to put some physics in to these criteria is still needed.

A lot of work was performed on modelling plasticity and oxidation with experimental verification on irradiated specimens with both observations of specimens and experiments in hot cells. Results showed that hardening is not sufficient from dislocation loop interaction. The development of interatomic potentials is more complicated than expected initially. Similarly, considerable amount of experimental tests on highly irradiated materials have been performed, however they were not fully profitable to the project as they were delivered with some delay (almost by the end of the project)

Concerning the user group, the objective was the evaluation of the platform tools by the non-developer users, with their own database. An important effort of the user group was dedicated to produce a comprehensive document reviewing the existing methods of predicting the effects of radiation on internals and RPV materials in all over the world.

The evaluation of simulation tools requires a collection of reference data (materials properties, conditions of irradiation, metallurgical evolutions, …) to be compared to predictions of the simulation tools, both for RPV and Internals materials. All these elements were gathered (with effort and time) in a specific database using the still existing PERFECT database and in close collaboration with the FP7 LONGLIFE project.

General Conclusions

The integrated project PERFORM 60, rich with its community that involves more than 350 scientists coming out from different disciplines has proven to be fairly effective in creating not only outstanding scientific and technical results as described above, but also to collaborate with each other in creating added value results for the European/international community. The project was also able to motivate an important number of end users, coming out from different horizons (constructors, utilities, safety organisations, ...) who showed great interest in the developed simulation tools and participated actively in their evaluation and dissemination of knowledge (see the section related to the dissemination). In addition the work done within the project has generated more than 100 scientific publications in international and peer reviewed journals and conferences which made the EU-community taking the leading role in the field.

The great success of the project is also translated by the fact that all deliverables and milestones have been achieved. Most importantly more than 20 young engineers have obtained PhD degree based on the work performed within the project in different European countries.

Last but not least, all the events organised by the project (more than 100 international participants in each of them) were a real happening in the scientific community.

Finally, this success story is not yet achieved as more collaborative work is needed to transfer the complex basic work performed within the last decade to more engineering oriented modelling tools that would help the nuclear industry better assessing the residual lifetime of the two very important and irreplaceable components, namely, the pressure vessel and its internals.

Acknowledgement

The author acknowledges the technical contributors, listed in annex 1, whose help was essential to achieve successfully PERFORM 60 project. The sponsoring of the European Commission to PERFORM 60, within the FP7 of Euratom for Nuclear Research and Training Activities, Theme 'Nuclear Fission and Radiation Protection' (Project number 232612), is also acknowledged.

Annex 1: List of scientific and technical contributors

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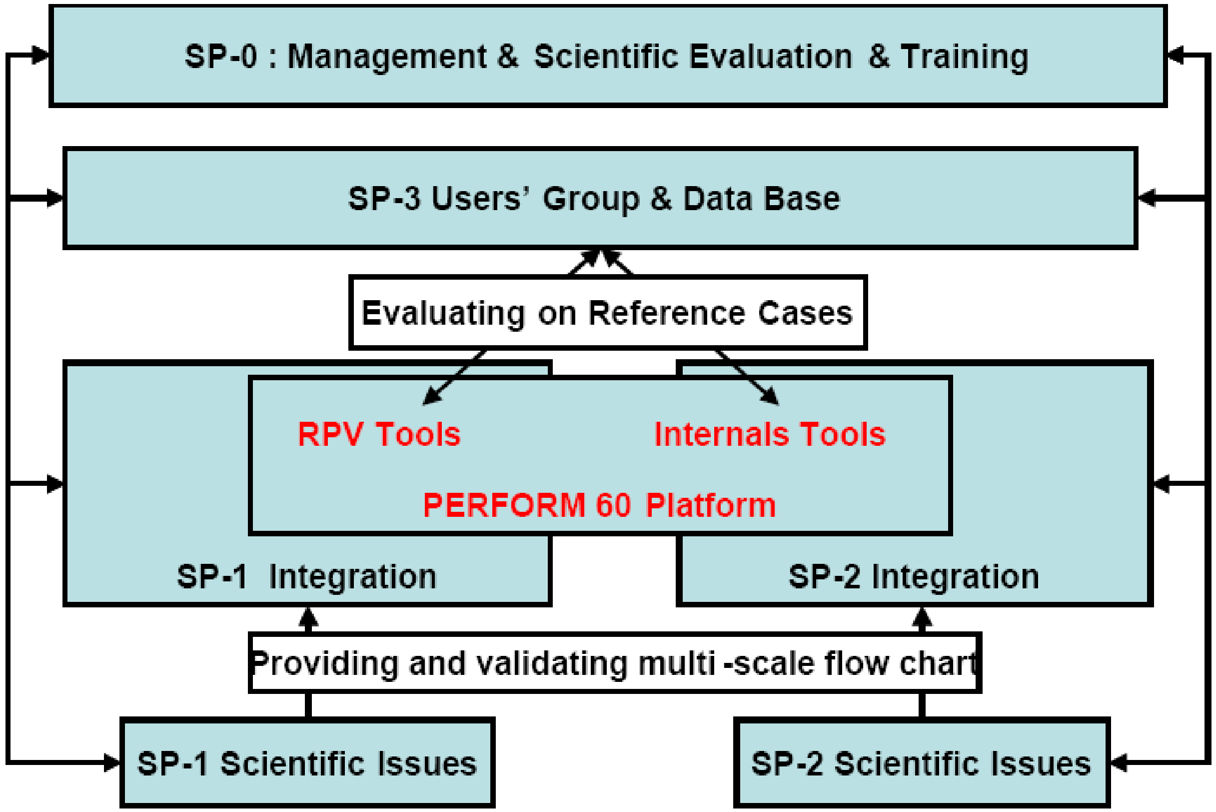


Figure 1 : Illustration of the work organisation within PERFORM60 project

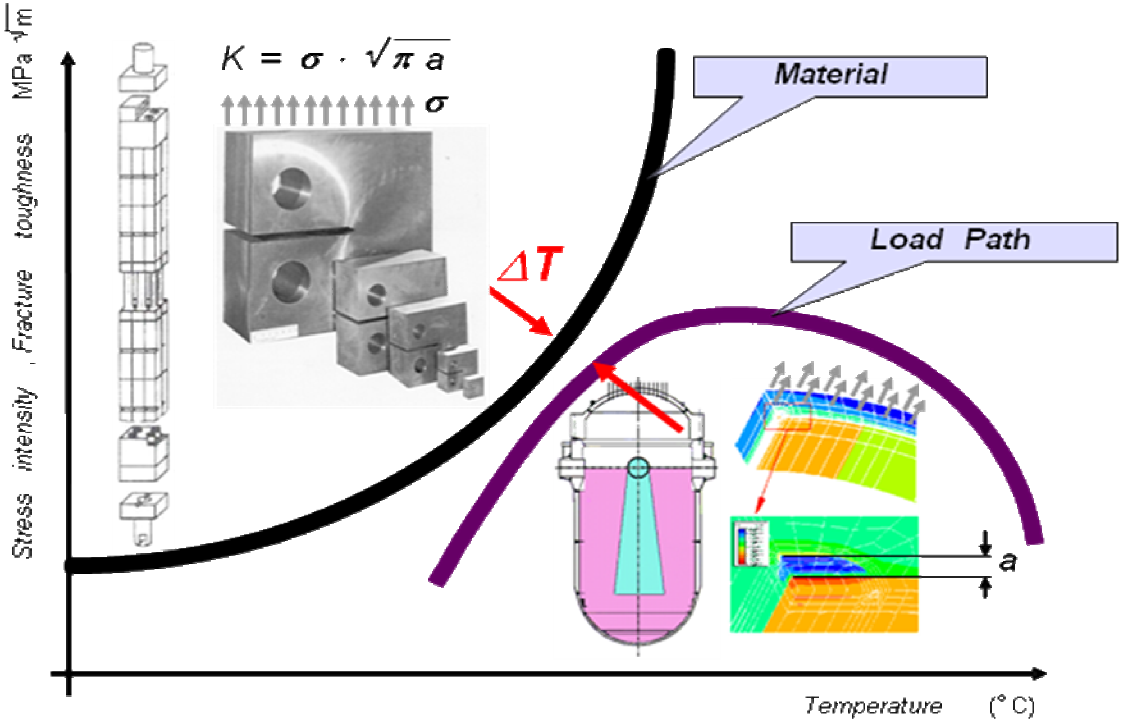


Figure 2: The irradiation-induced shift (ΔT) in the brittle to ductile transition temperature for current RPV steels determined from surveillance programmes (top left) should not exceed the load path (estimated from various transient analysis) in order to avoid brittle fracture.

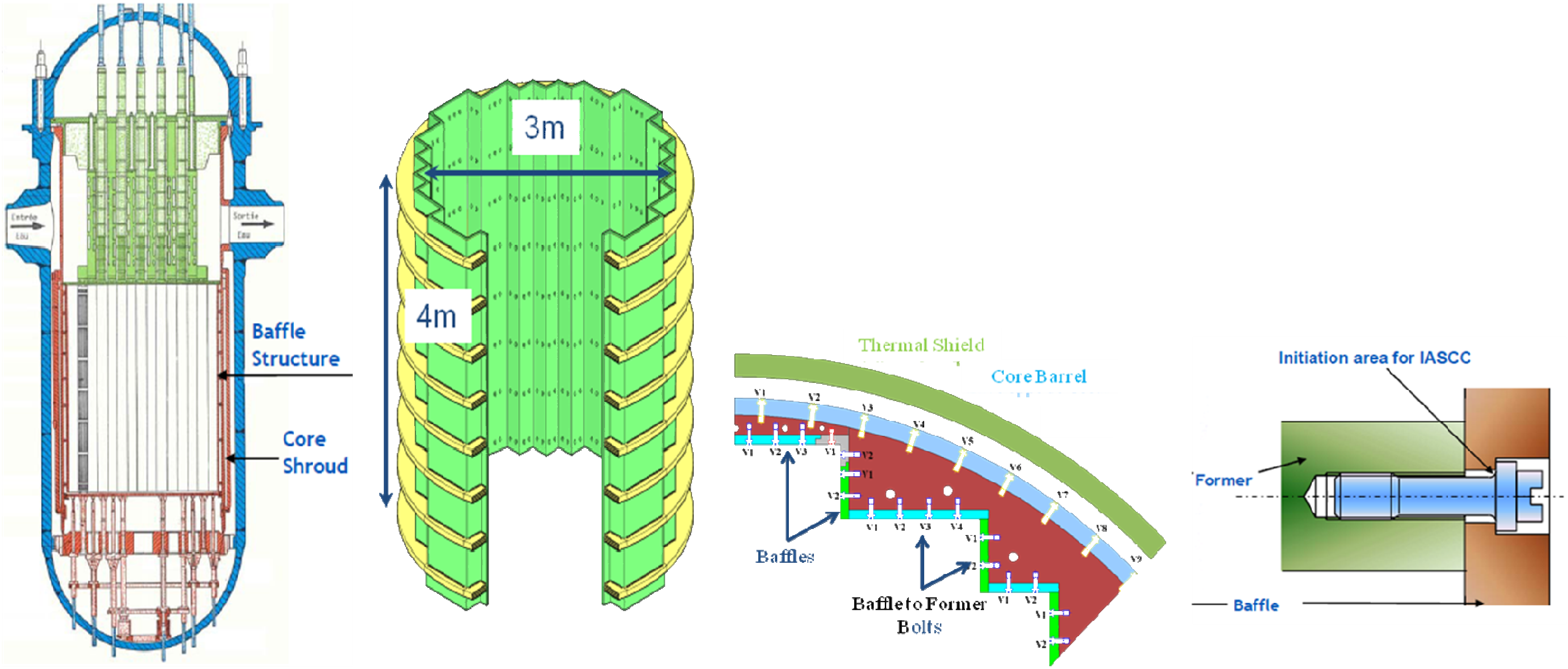


Figure 3: Internals components studied within the project

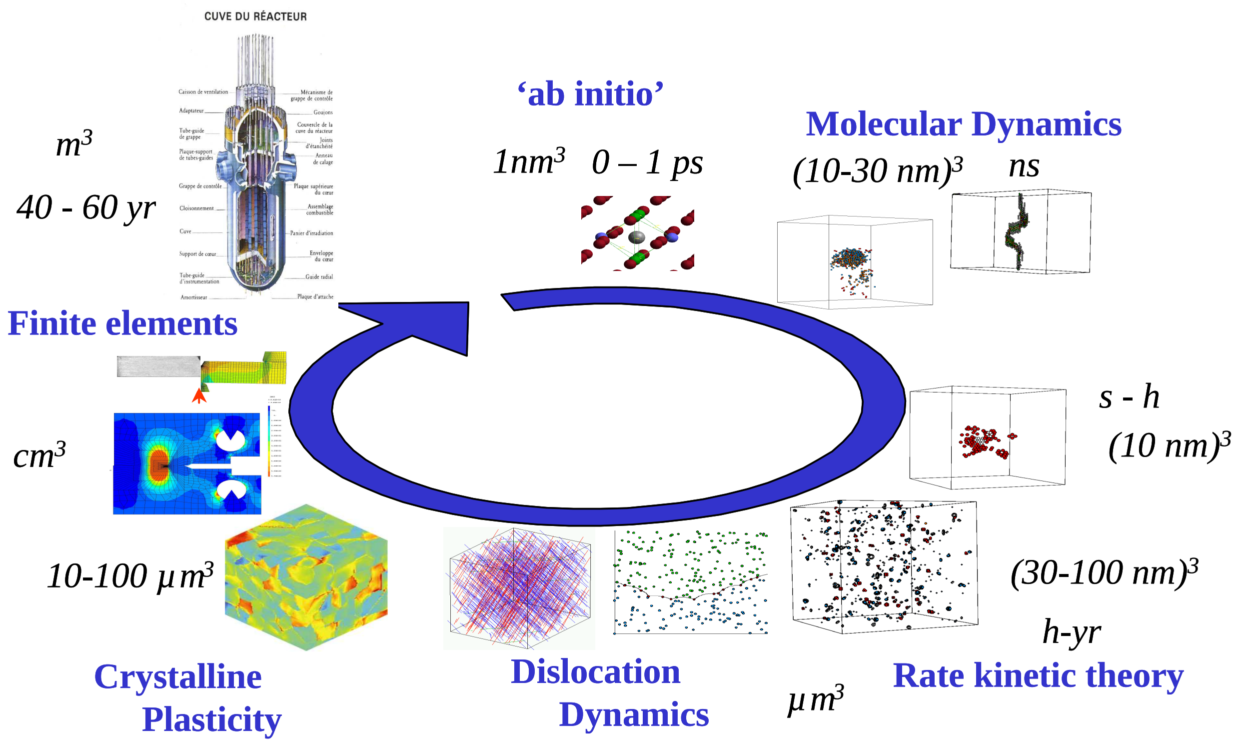


Figure 4: The multi-scale approach adopted to simulate the behavior of RPV steel within FP6-PERFECT project

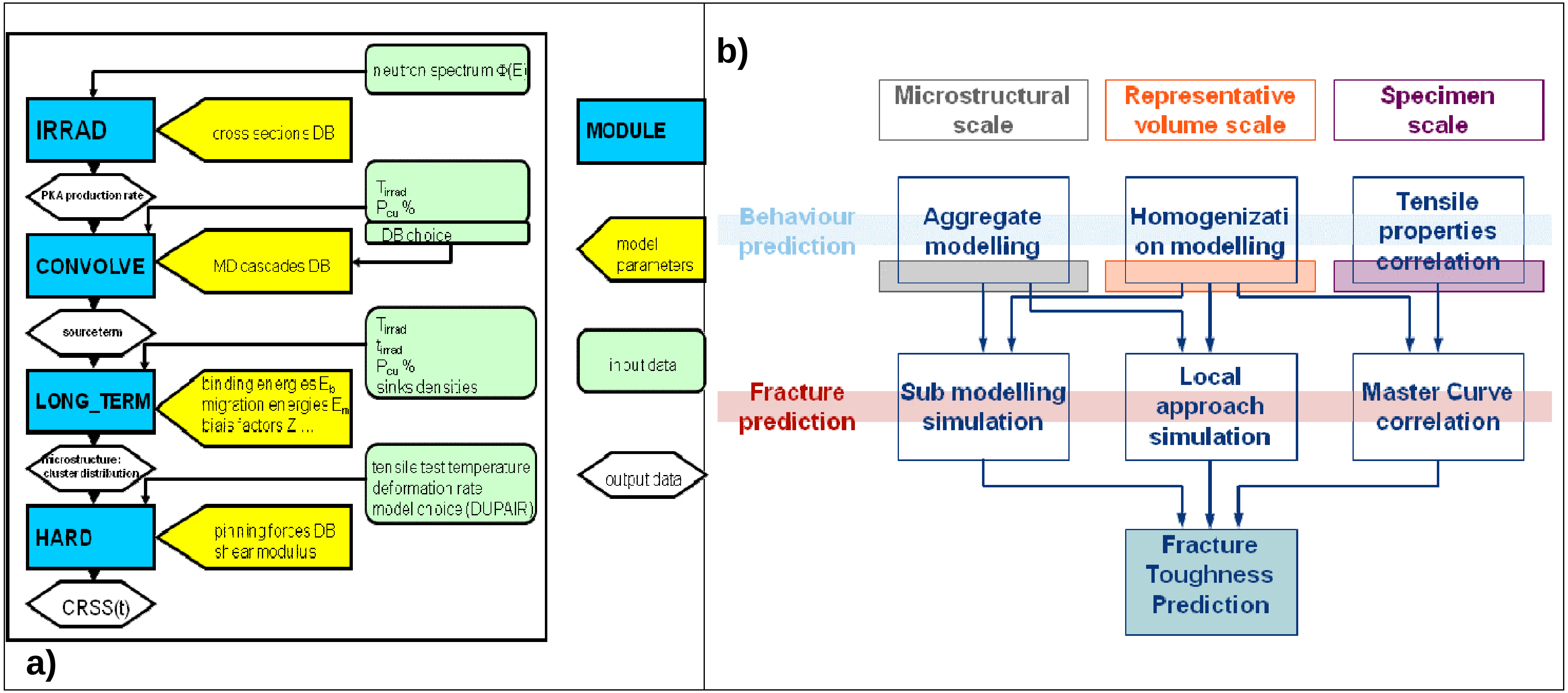


Figure 5: The chain of modules needed to develop the end products: a) microstructure and hardening (RPV-2), b) Fracture toughness (Thoughness) as envisaged during the FP6-PERFECT project.

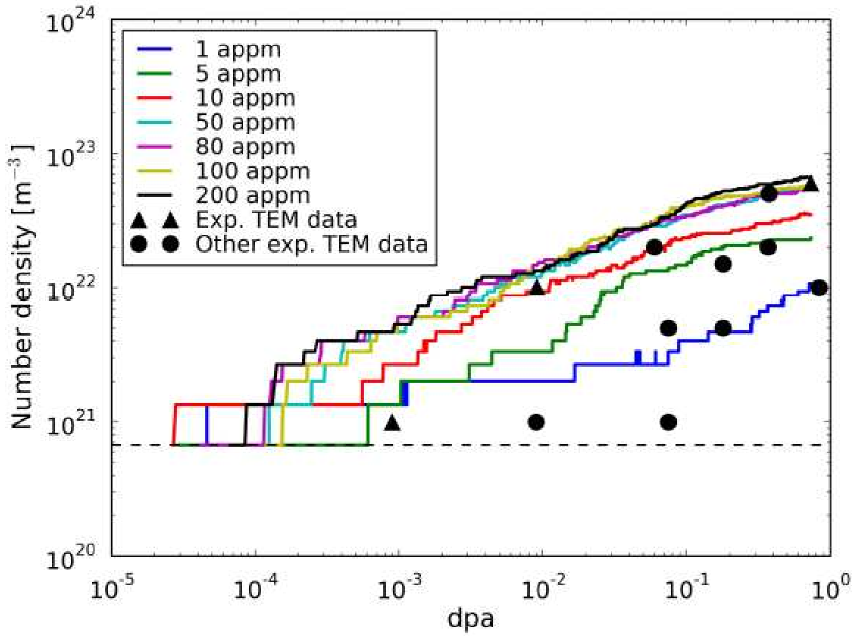


Figure 6 – Effect of the concentration of traps (which correlates with the concentration of C atoms in the matrix) on the evolution of the number density of visible loops with increasing irradiation dose. Note that an effect becomes visible only for extremely low concentrations, while increasing concentrations lead to a saturation of the effect.

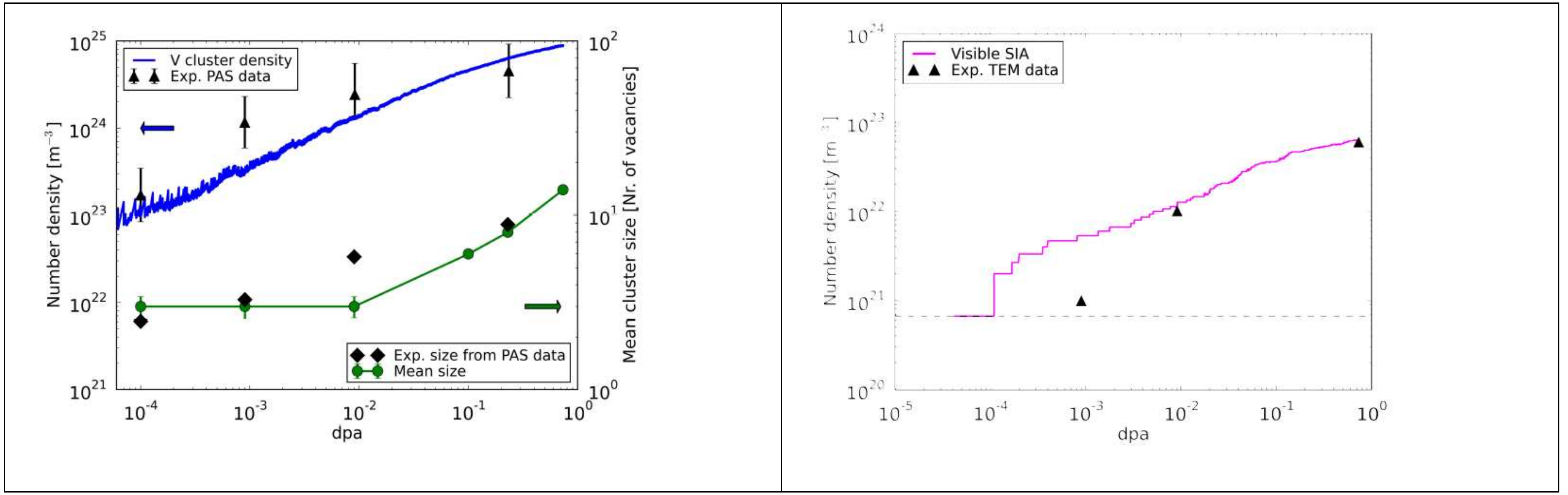


Figure 7 – Left: evolution with dose of density and mean size of vacancy clusters in Fe-C, according to the OKMC model and in the experiment (PAS). Right: evolution with dose of the density of visible SIA clusters (loops), according to the OKMC model and in the experiment (TEM). Irradiation temperature (=340 K); dose-rate (~10^{-7} dpa/s). The overestimation of loop density at low dose is probably due to the fact that traps exist in the model since the beginning, while in reality they form progressively (carbon-vacancy complexes).

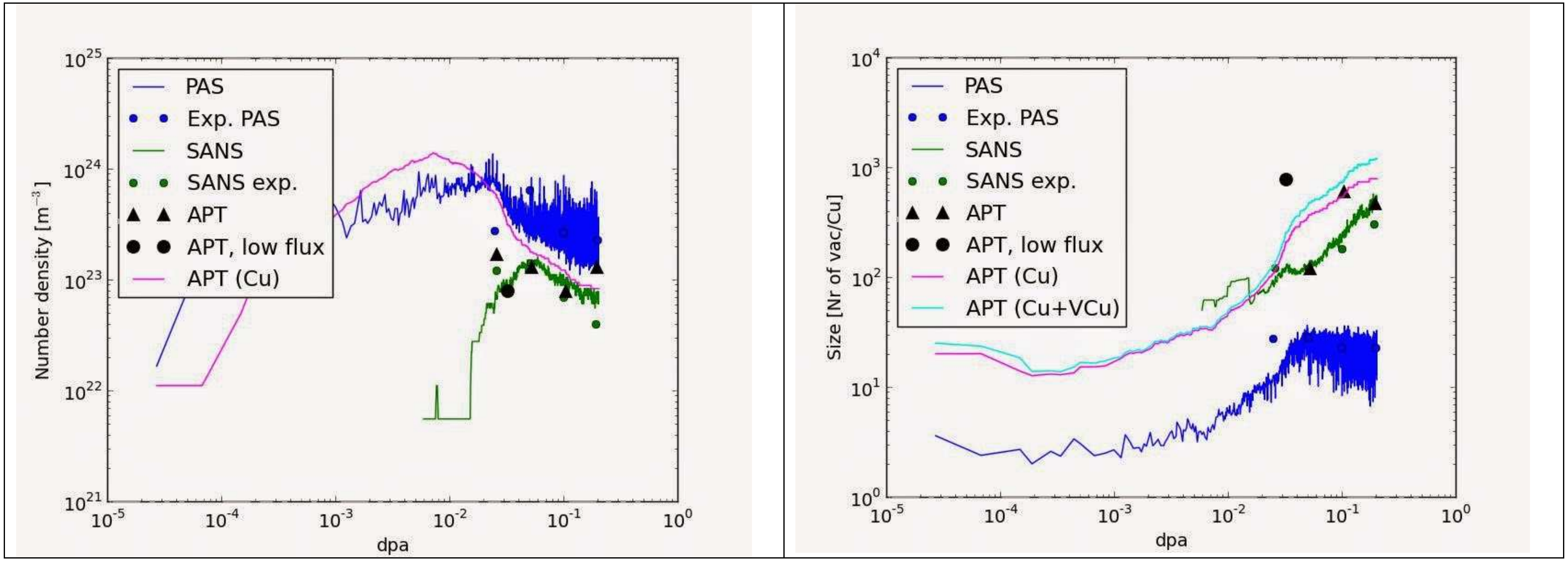
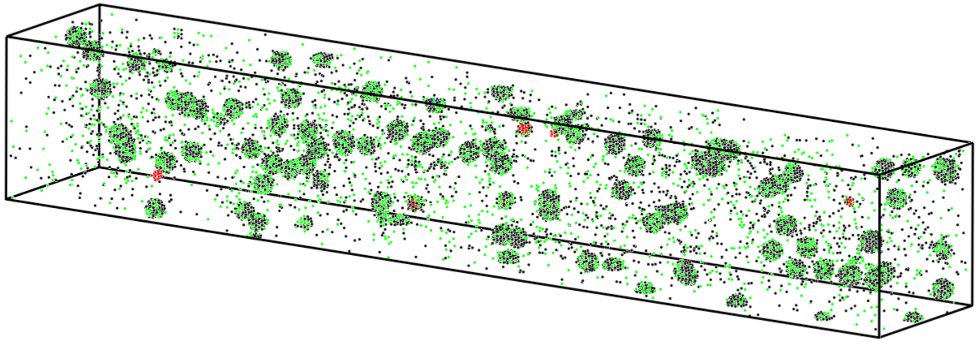


Figure 8– Results of the OKMC model for FeCuC allosy at RPV operation temperature. Left: number density, and right, mean size (nr of Cu atoms and/or vacancies) of Cu precipitates (Cu-vacancy clusters), counted according to different criteria, to match what PAS, SANS and APT can see.



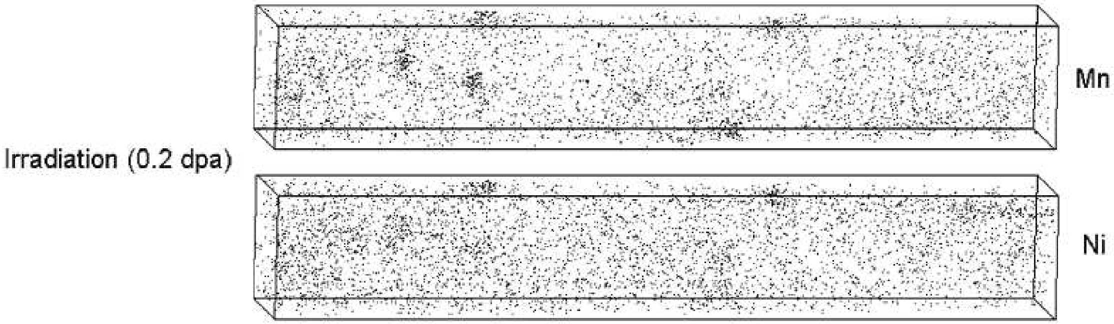


Figure 9: Above: snapshot of the simulation box including vacancies (blue), SIAs (red), Mn (black) and Ni (green) at 0.2 dpa: high density of MnNi rich clusters is clearly visible. Below: comparable volume from atom probe examination of FeMnNi alloys irradiated at the simulated conditions.

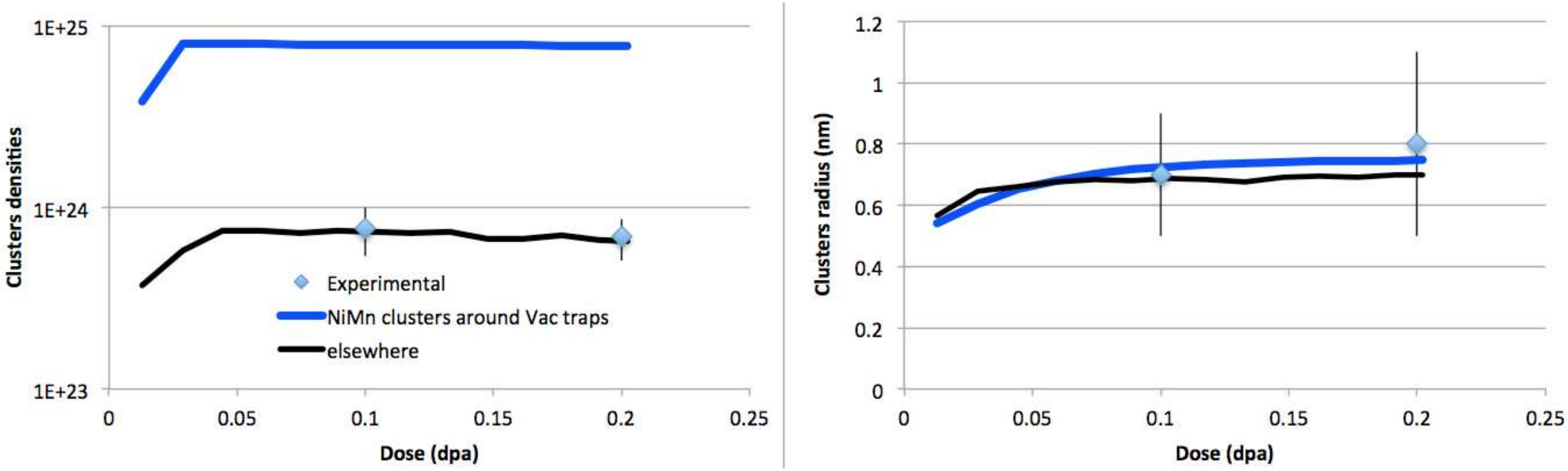
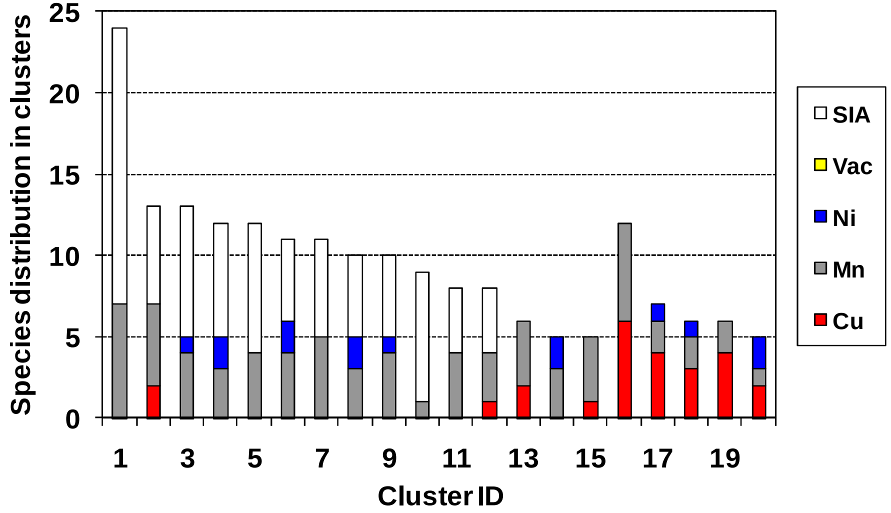


Figure 10: Evolution with dose of Ni-Mn clusters density (left) and radius (right) distinguishing between clusters formed: around generic traps for vacancies; (b) elsewhere in the simulation box (on SIA clusters).



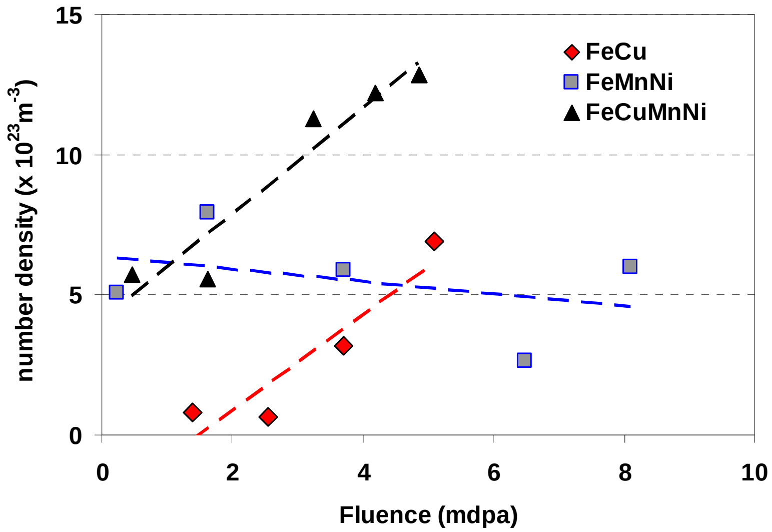


Figure 11 - Left: composition of clusters formed in the FeNiMnCu alloy: two families (with Cu and nd without Cu but with self-interstitial atoms) are clearly distinguished. Right: evolution of number density of clusters with dose in the different alloys (note that only very low dose could be simulated).

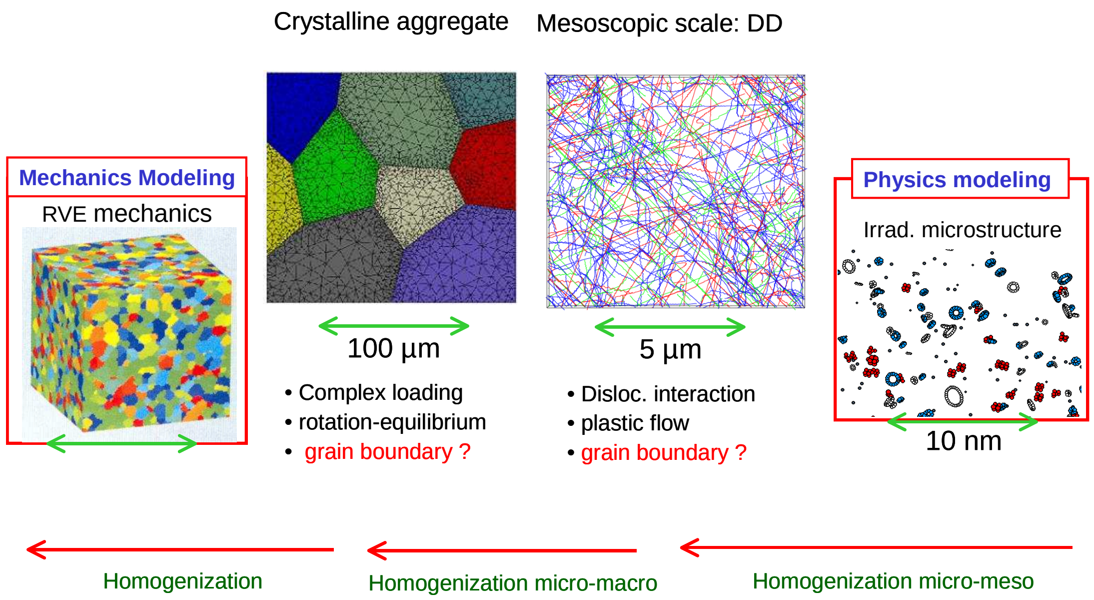


Figure 12: Scheme used to model the flow properties of RPV steel.

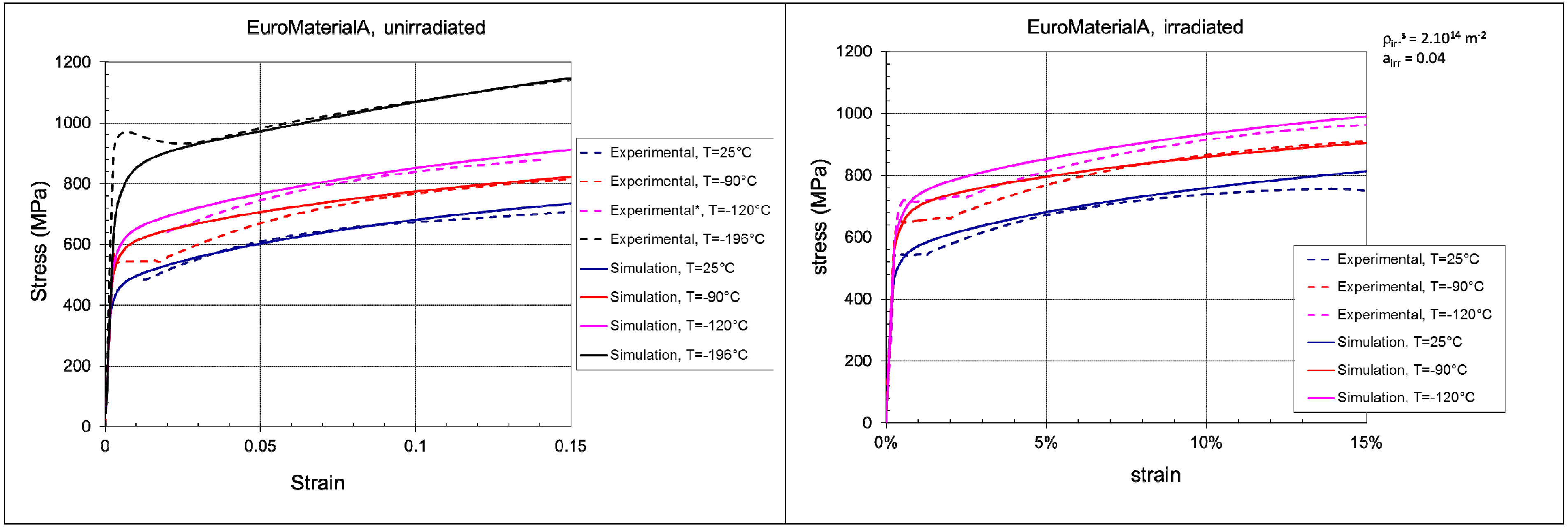


***Figure 13**: Comparison of the experimental and computed tensile curves at different temperatures for the un-irradiated and irradiated conditions. Material is the Euromaterial A.*

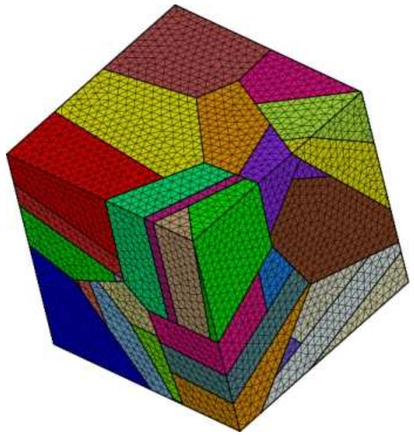


Figure 14: *Typical microstructure mesh (10 parent grains, 5 lath packets) built using the developed software.*

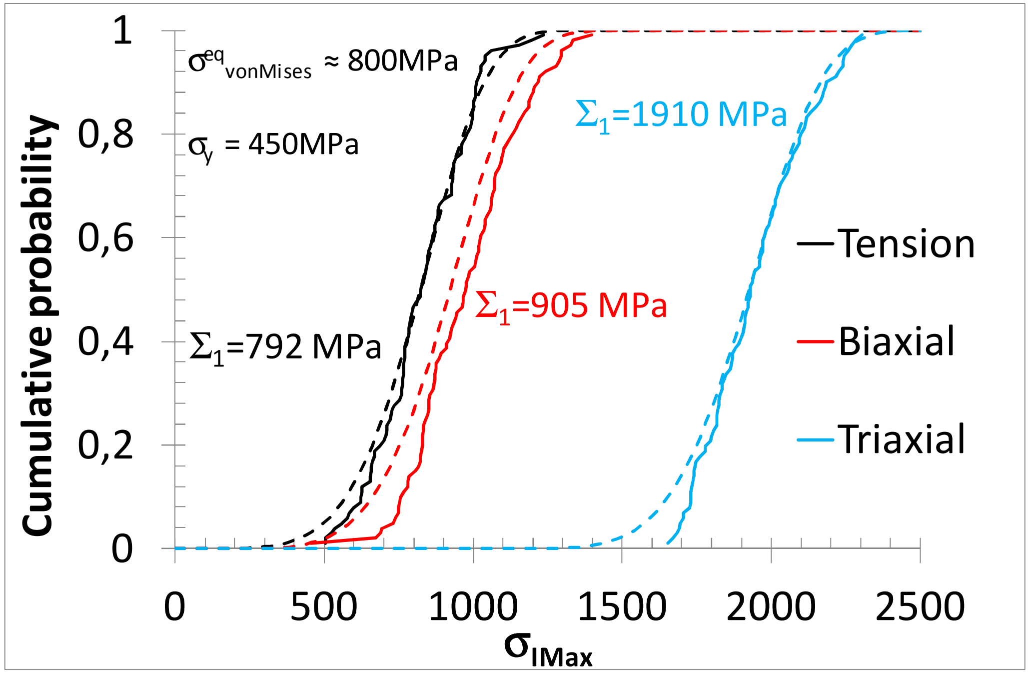


***Figure 15**: Maximum principal stress distributions in the bainitic packet for the uniaxial, biaxial and triaxial loadings for von Mises stresses close to 800 MPa.*

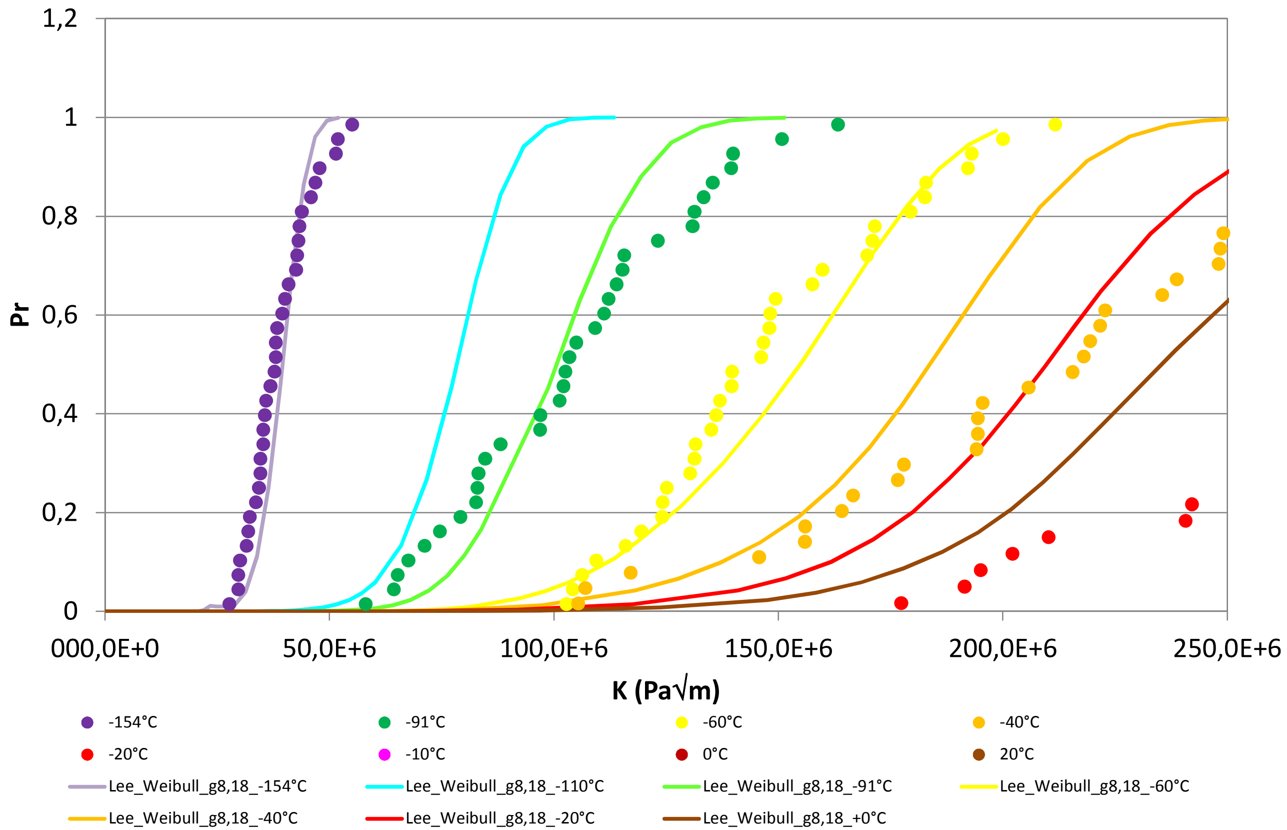


Figure 16: Comparison between MIBF model results for γ_f = 8.18 J/m^2 and experimental fracture toughness results for 1T C(T) specimen

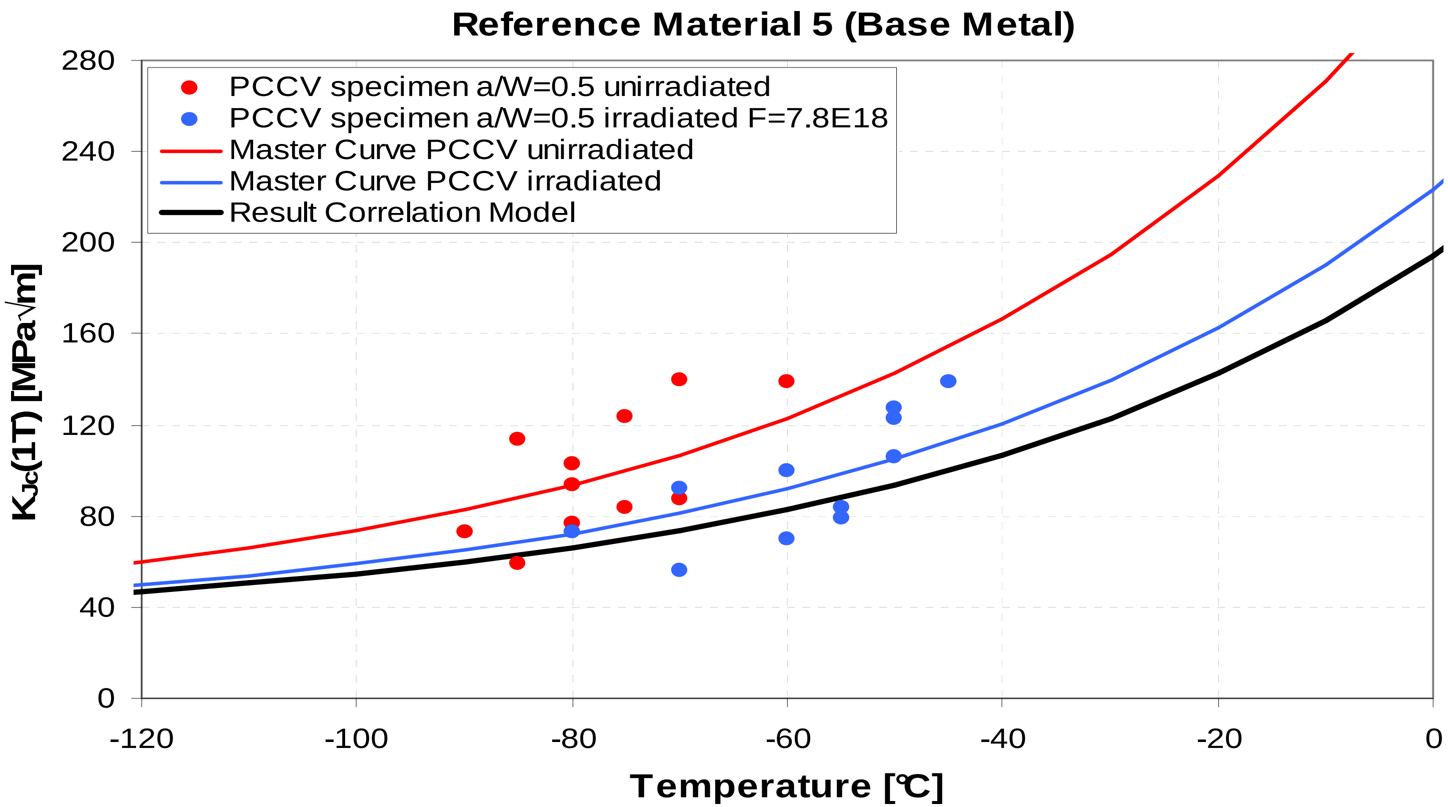


Figure 17: The irradiated fracture toughness curve (black) is predicted from the unirradiated data (red) and yield stress change using the Beremin model. Results are in good agreement with the irradiated data (blue).

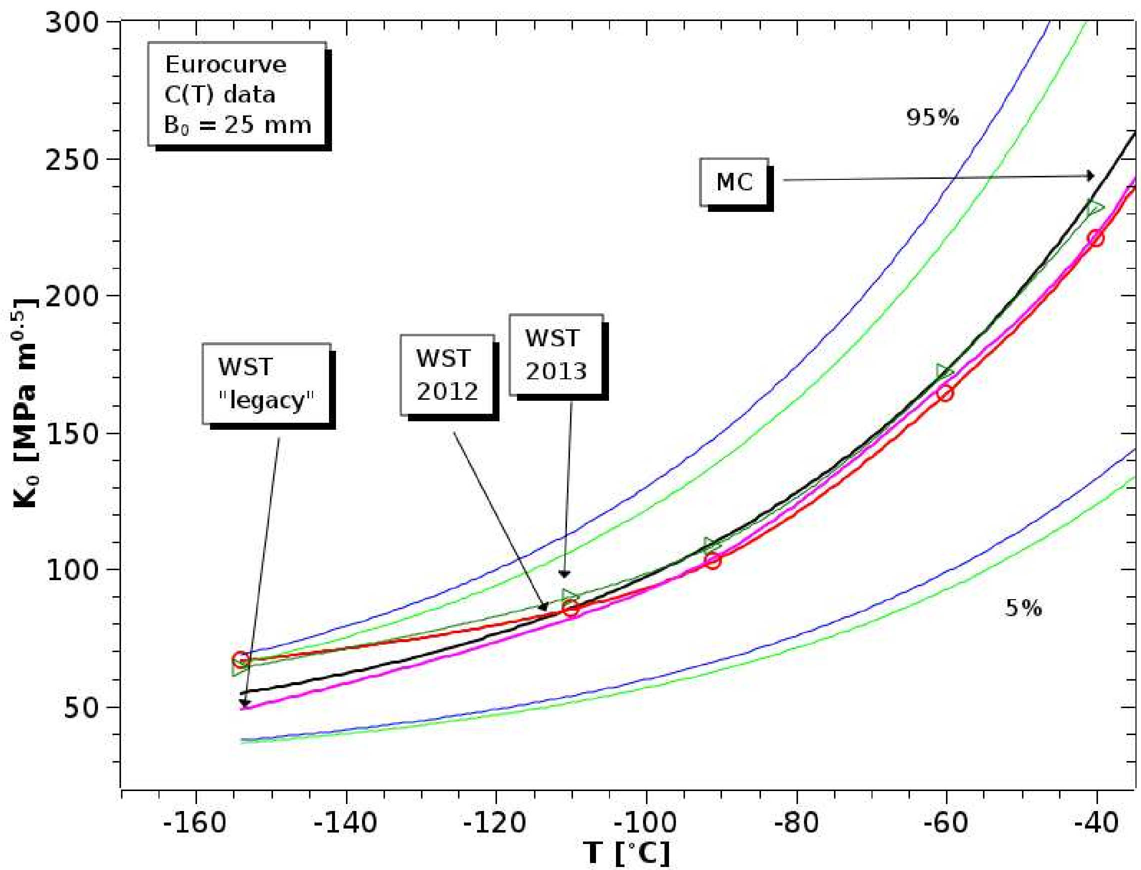


Figure 18: application of WST model (with the different versions developed during the project: WST2012, WST2013) to the Eurocurve 'Material A' data

Figure 19: summary of the progress made from PERFECT to PERFORM60

PERFECT (2007)	PERFORM (today)
- Irradiation damage in Fe; - Microstructure evolution under irrad. FeCu: homogeneous precipitation (MFVISC); - Hardening (micro-cavities, Cu-rich clusters) - Flow behavior: emperical plasticity law; - FTM: local approach (Beremin type based on the homogenization of a microstructure of Voronoi type; - Plateform: Perspycace/ Python Qt3 - UG: database on fracture/ application as demonstration	- Irradiation damage based on annealed MD (BC) cascades - Microstructure: heterogeneous precipitation (CRESCENDO) - Interatomic potentials : FeCuNiC, FeNiMn (1 aprrox.) - Hardening: various defect/solute clusters (VC, NiCuV, decorated loops, …) (validated on real steels) - Coupling between hardening and advanced fracture models - Cristal plasticity laws based on DD - Experimental validation at the appropriate scale (mono-crystal, grain, poly, …) - Homogenization and aggregate calculations on bainitic structure - advanced cleavage models : Beremin, WST, Bordet, MIBF

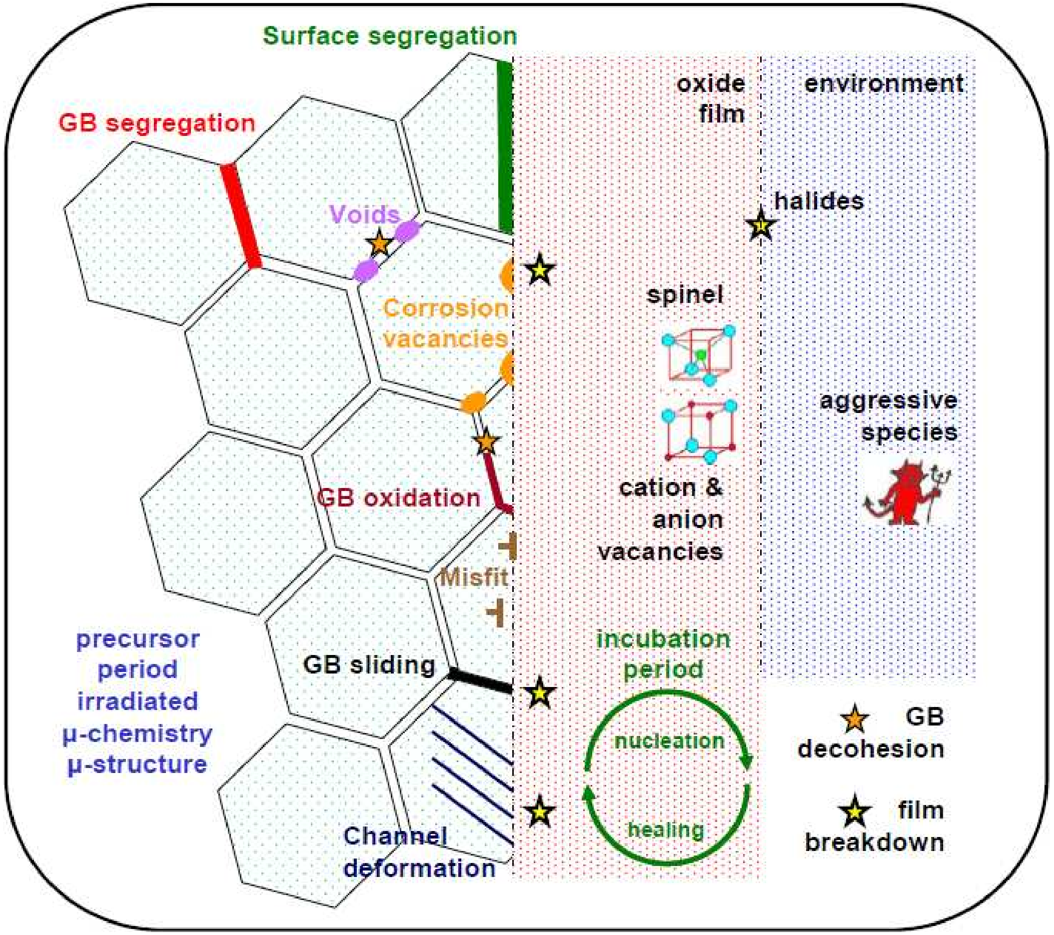


Figure 20: schematic illustration of the interaction of the water coolant with an internal component in PWR.

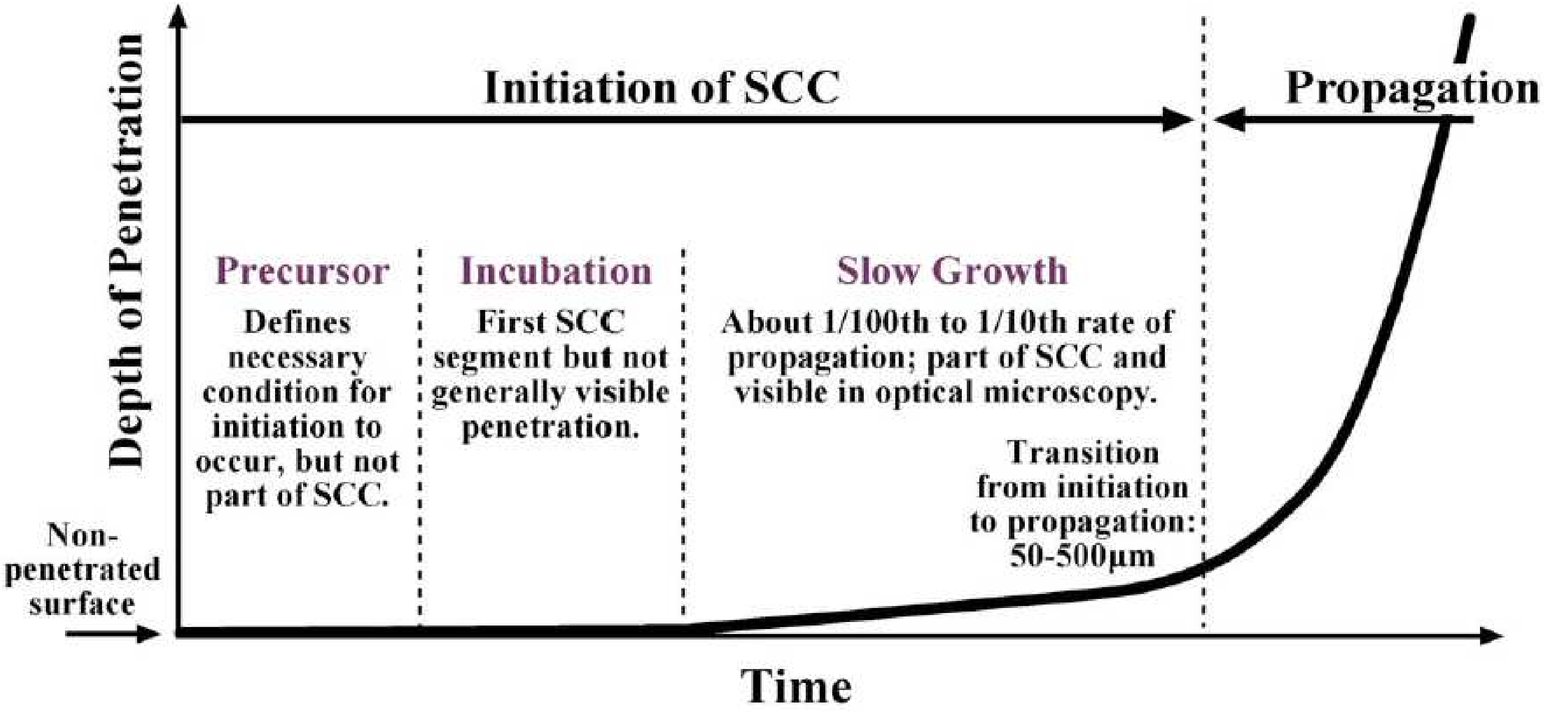


Figure 21: Precursor, incubation, slow growth and propagation description of the development of a stress corrosion crack

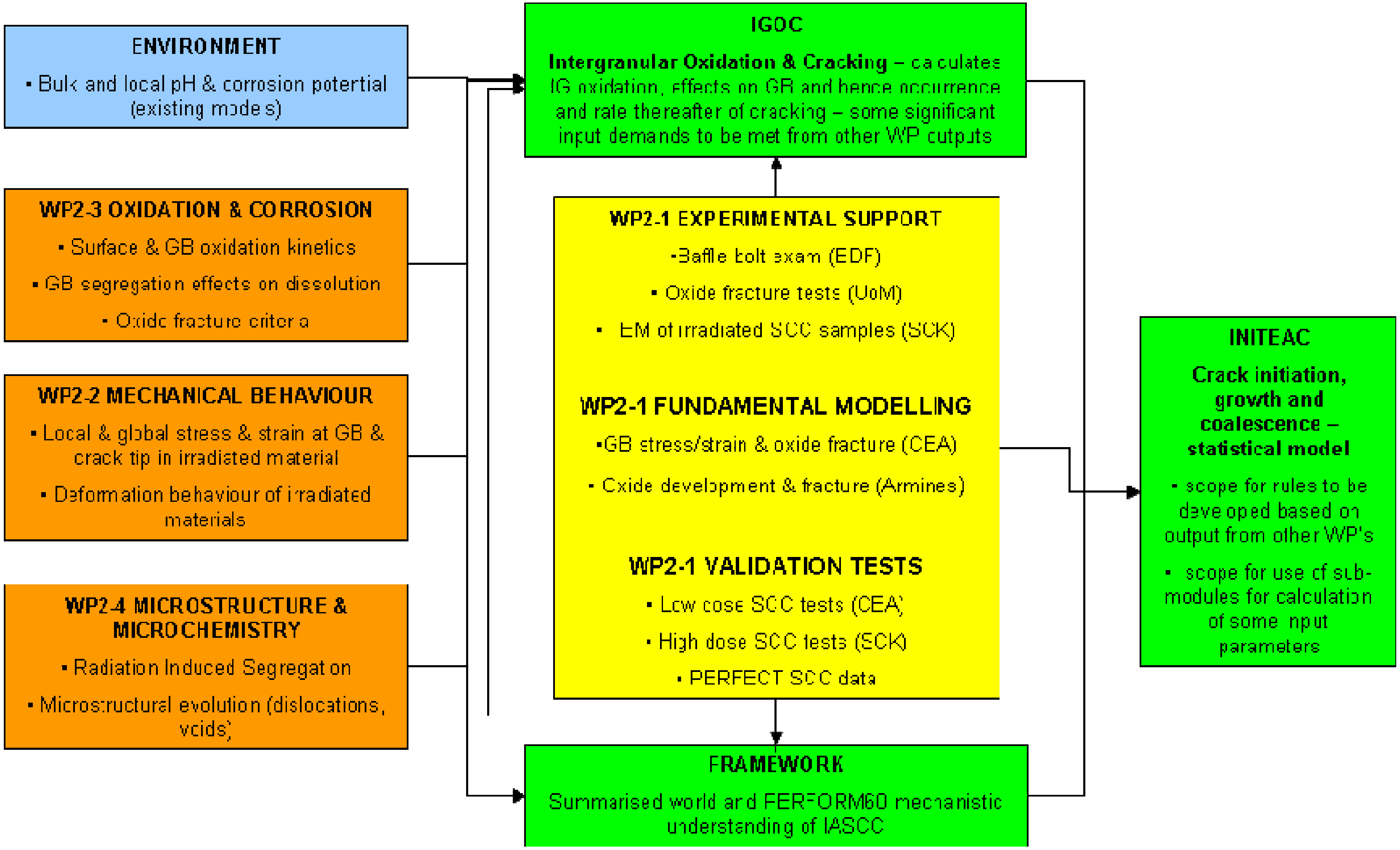


Figure 22: Inter-dependency between the models developed in SP2

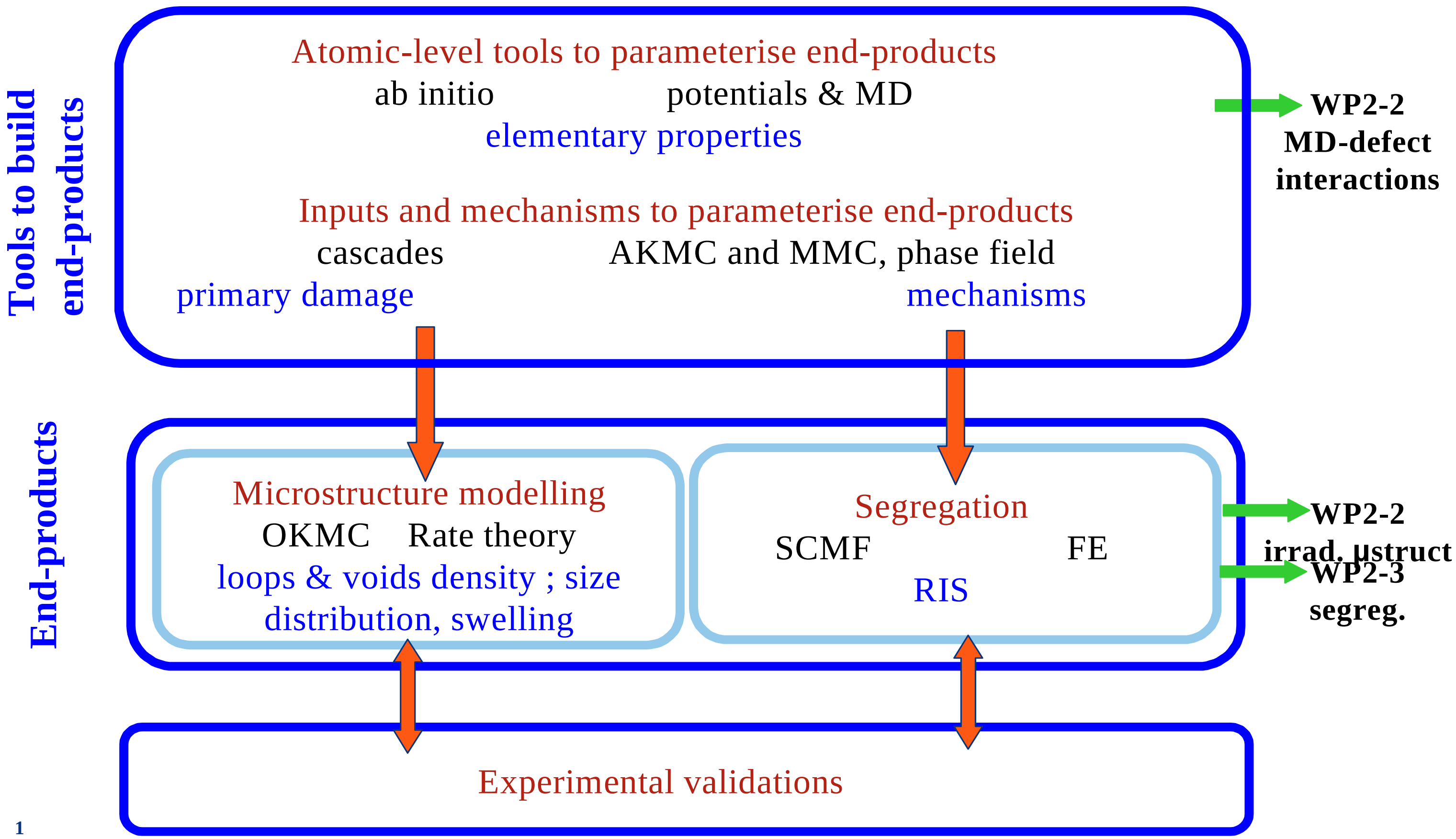


Figure 23: steps followed to produce the INTERN end product

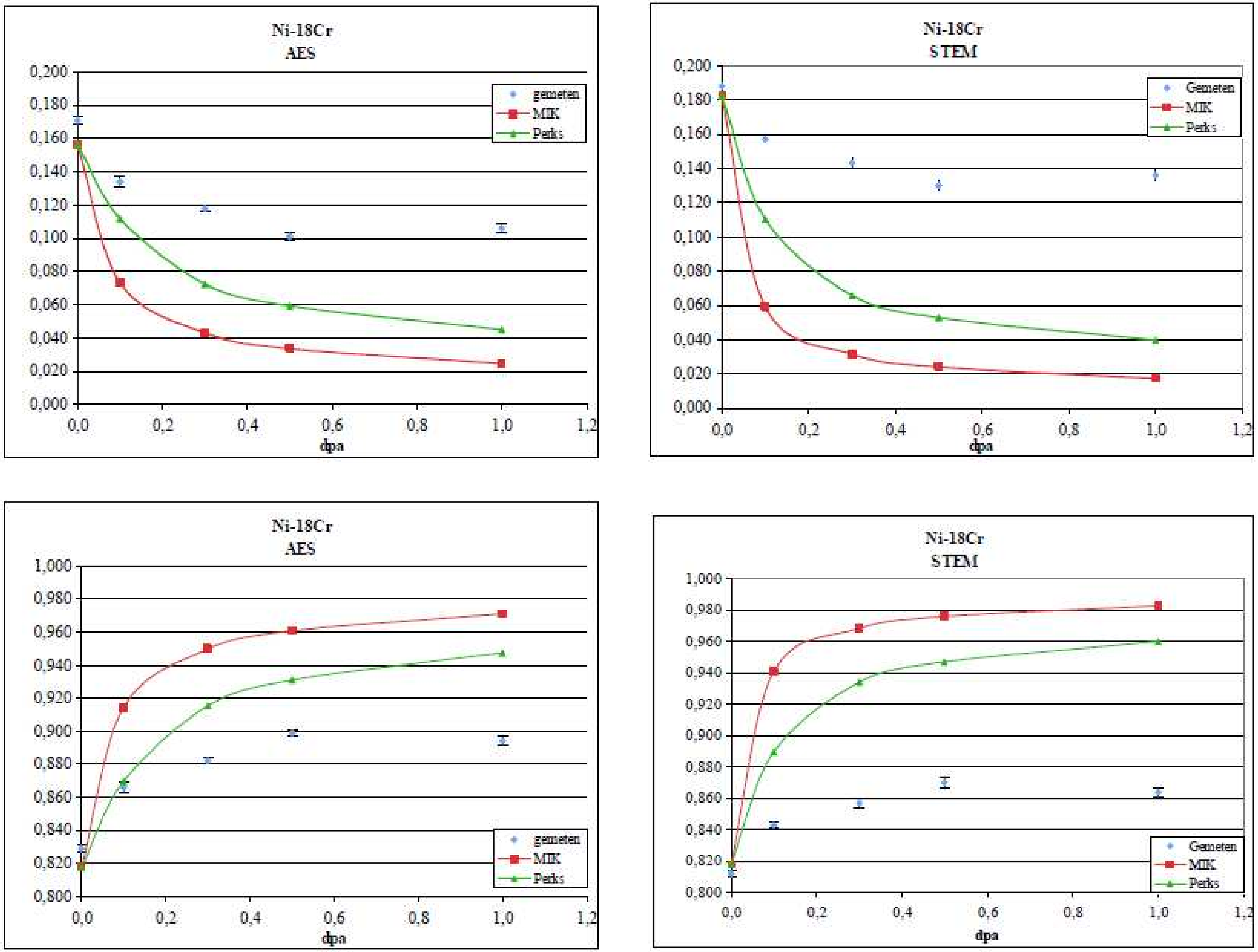


Figure 24: Comparison between measured and calculated grain boundary concentrations for chromium (top) and nickel (bottom) versus fluence for Ni-18Cr; AES (left) (left) and STEM (right). Proton flux 7 10^{-6} dpa/s at 400°C.

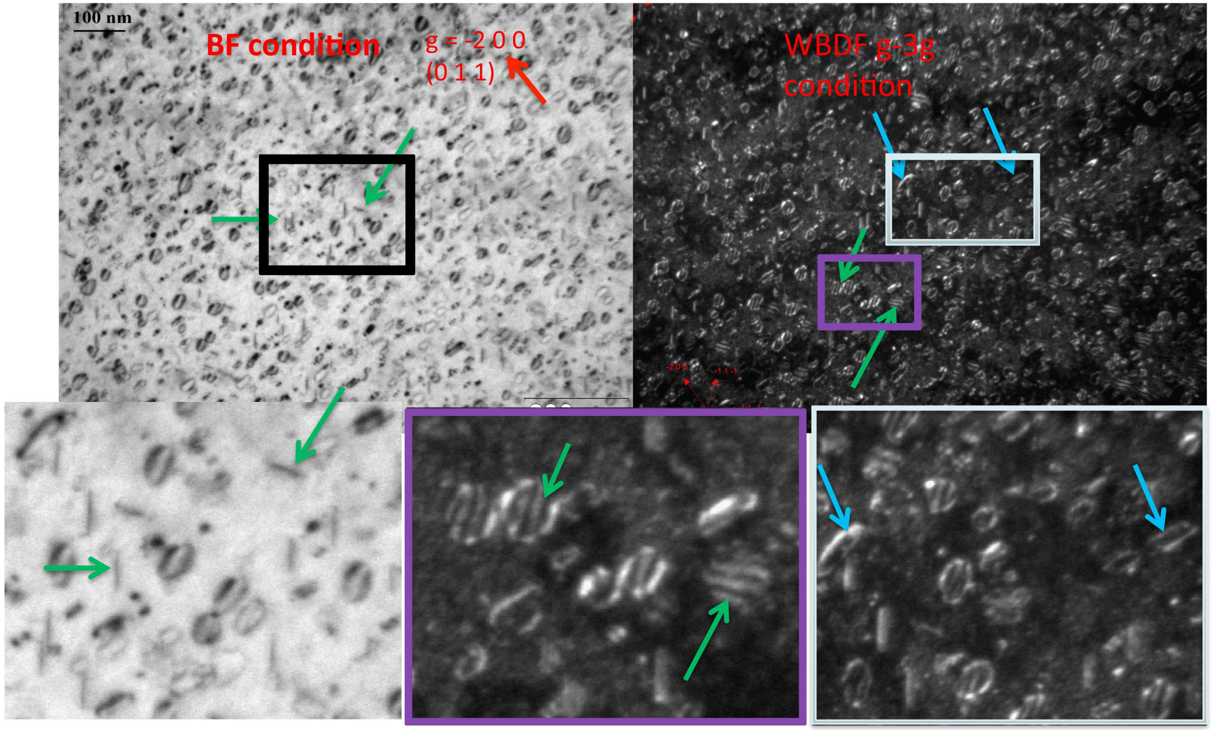


Figure 25*:* *316L* steel irradiated at 5dpa (450°C 5MeV Ni2+ions). Green arrows: Frank loops (4 families) Blue arrows: Perfect loops

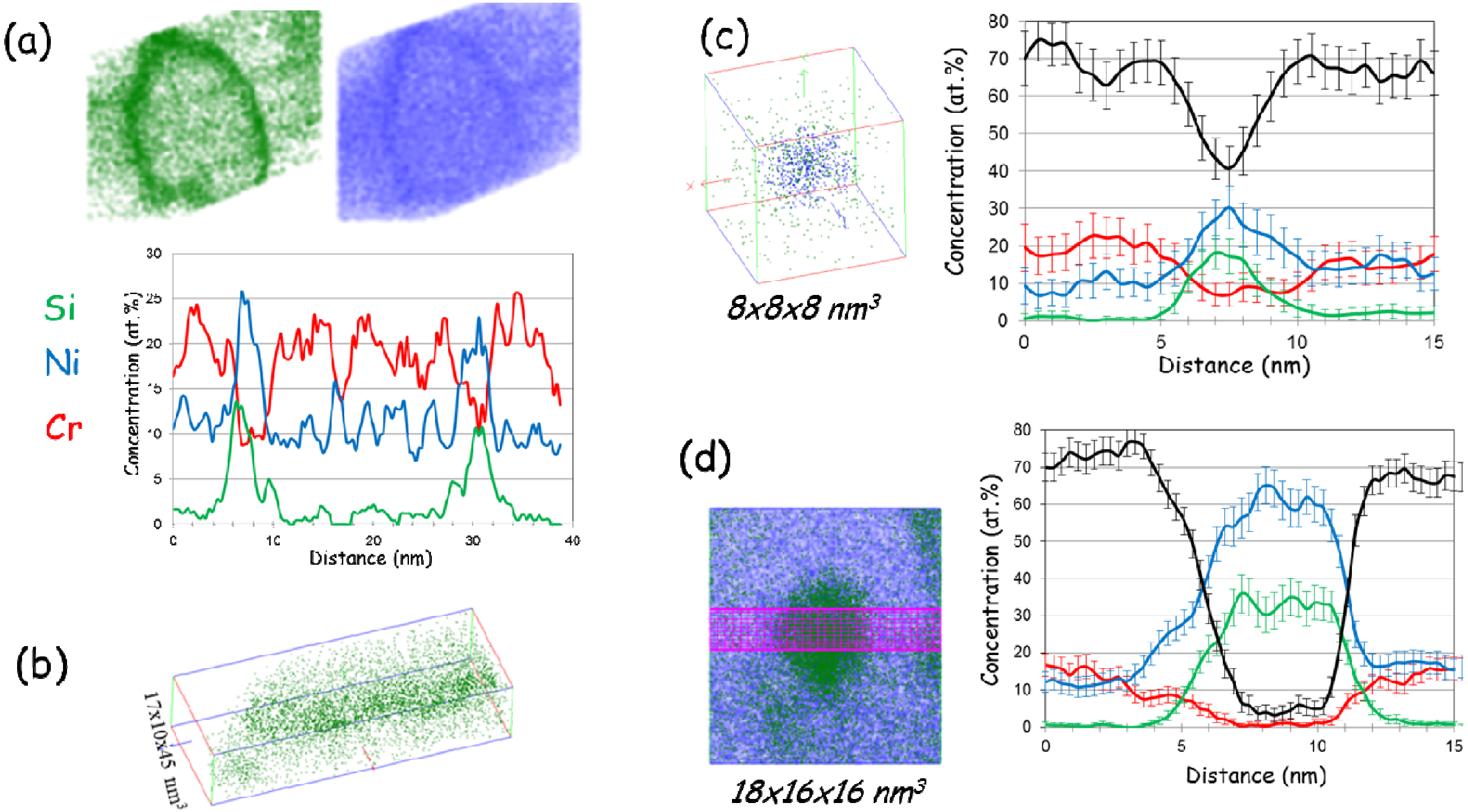


Figure 26: Summary of the different objects detected by APT. (a) and (b) Segregation along the lines of dislocation loops and straight dislocations respectively. (c) Solute (Ni, Si and/or P) clusters, have a peaked composition profile without plateau region. (d) Precipitates, have a similar shape than the clusters, but the composition profile exhibits a plateau and the level of Ni+Si is above 40 at.%.

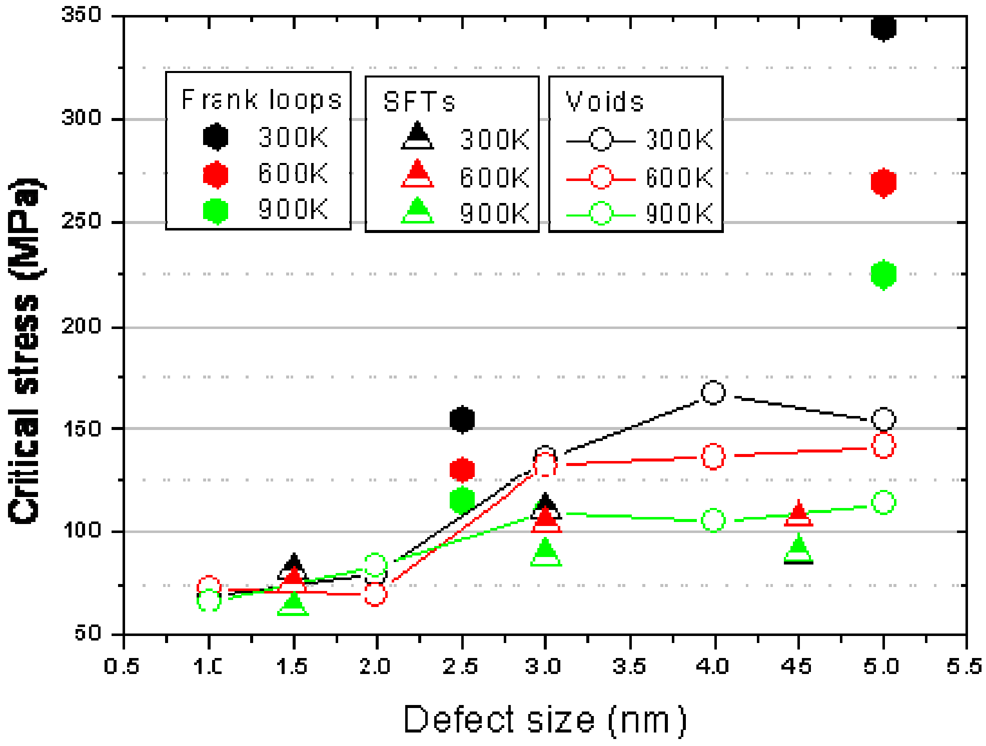


Figure 27: Comparison of critical stress level resulting from interaction between screw dislocation and SFT , void and Frank loop for different defects diameter at 300K, 600K, 900K .

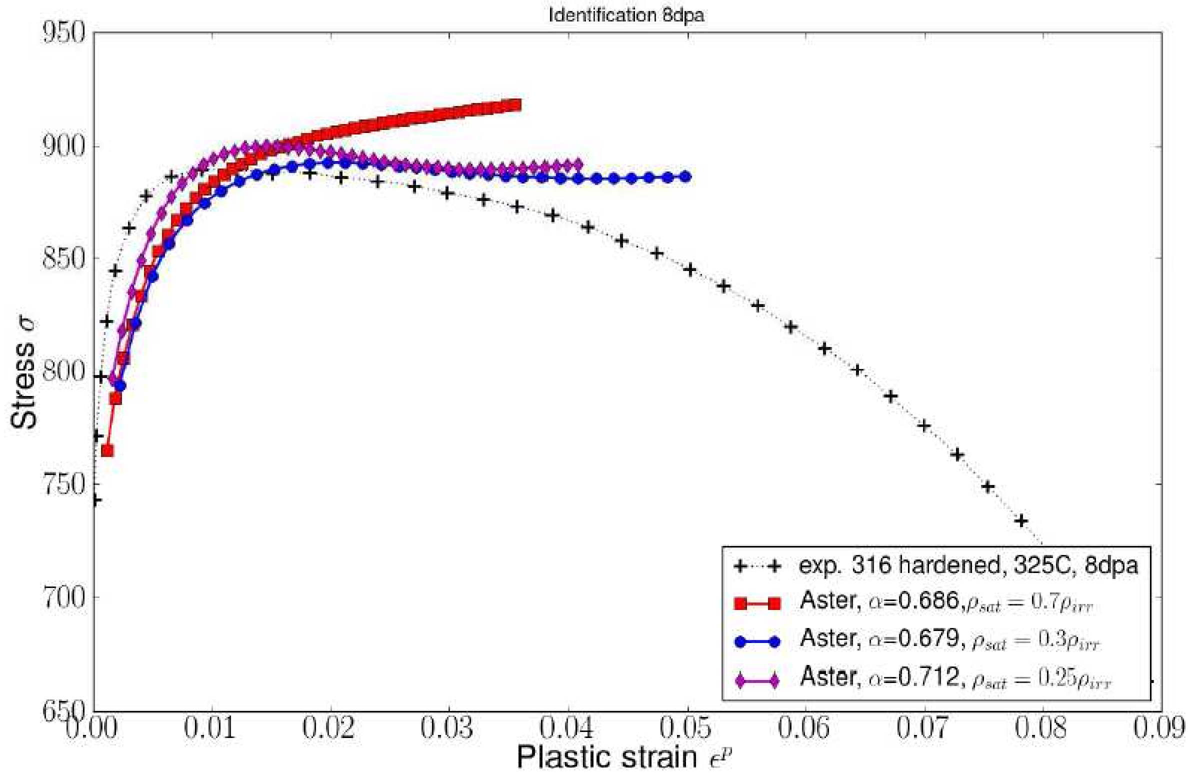


Figure 28: Macroscopic plastic response from the simulations based on a Berveiller-Zaoui homogenization procedure compare to the experimental results obtained from testing of irradiated state stainless steel to 8 dpa at 325°C.

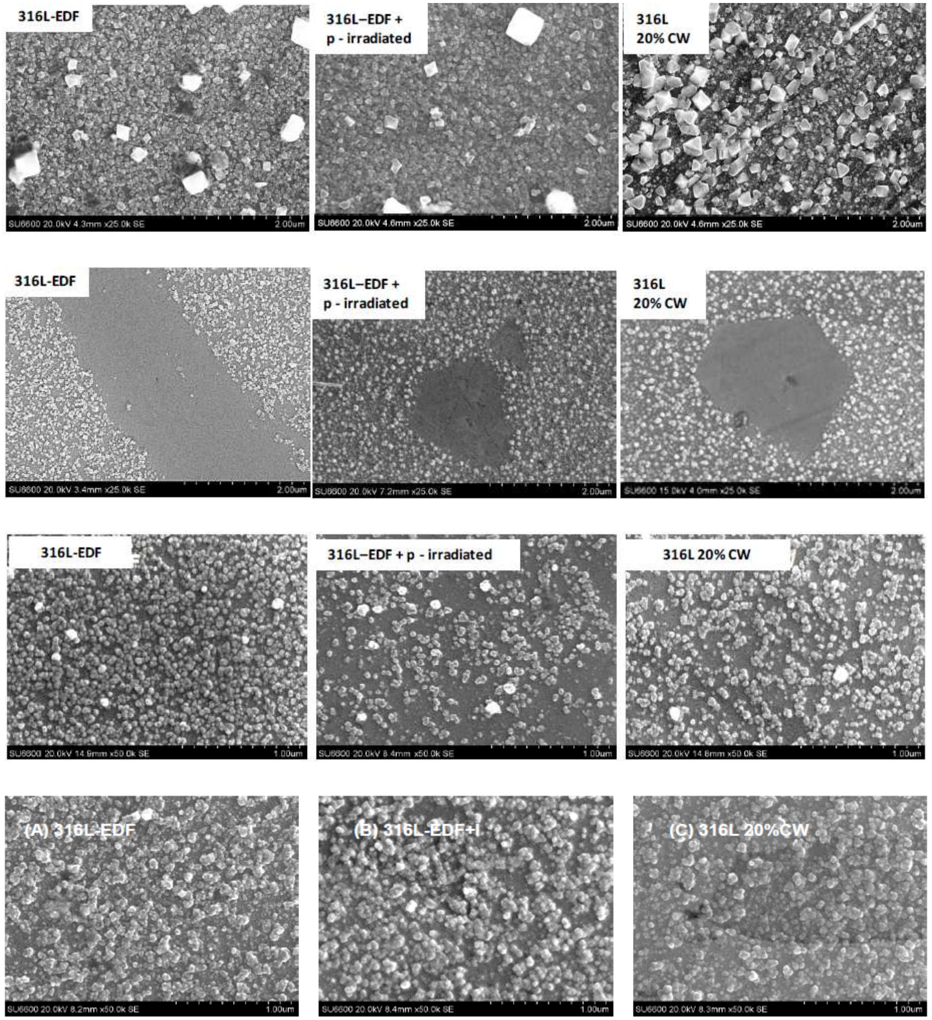


Figure 29: Long-term exposures to variations of PWR chemistry was apparently more sensitive to the particular conditions than to whether or not the material was proton irradiated or cold worked. top row: pH 7, 325 °C, 330 hrs; second row from top: pH 9, 325 °C, 330 hrs; second row from bottom: pH 7, 200°C, 1000 hrs; bottom row: pH 9, 200 °C, 1000 hrs.

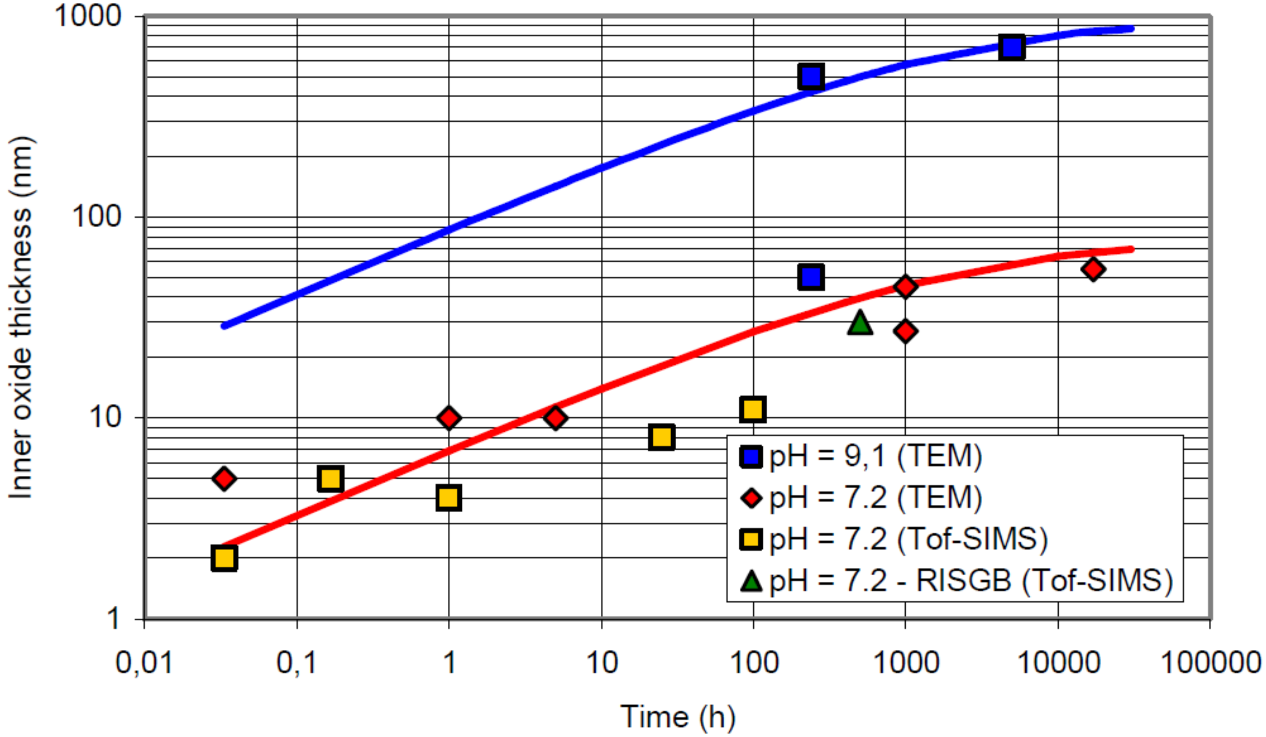


Figure 30: Development of inner, Cr-rich oxide layer with time on 316L SS exposed to PWR conditions, which clearly becomes much thicker at a pH of 9.1 versus 7.2. The GB-RIS model alloy was not distinctly different. The solid lines are predictions by KINOXID (EDF).

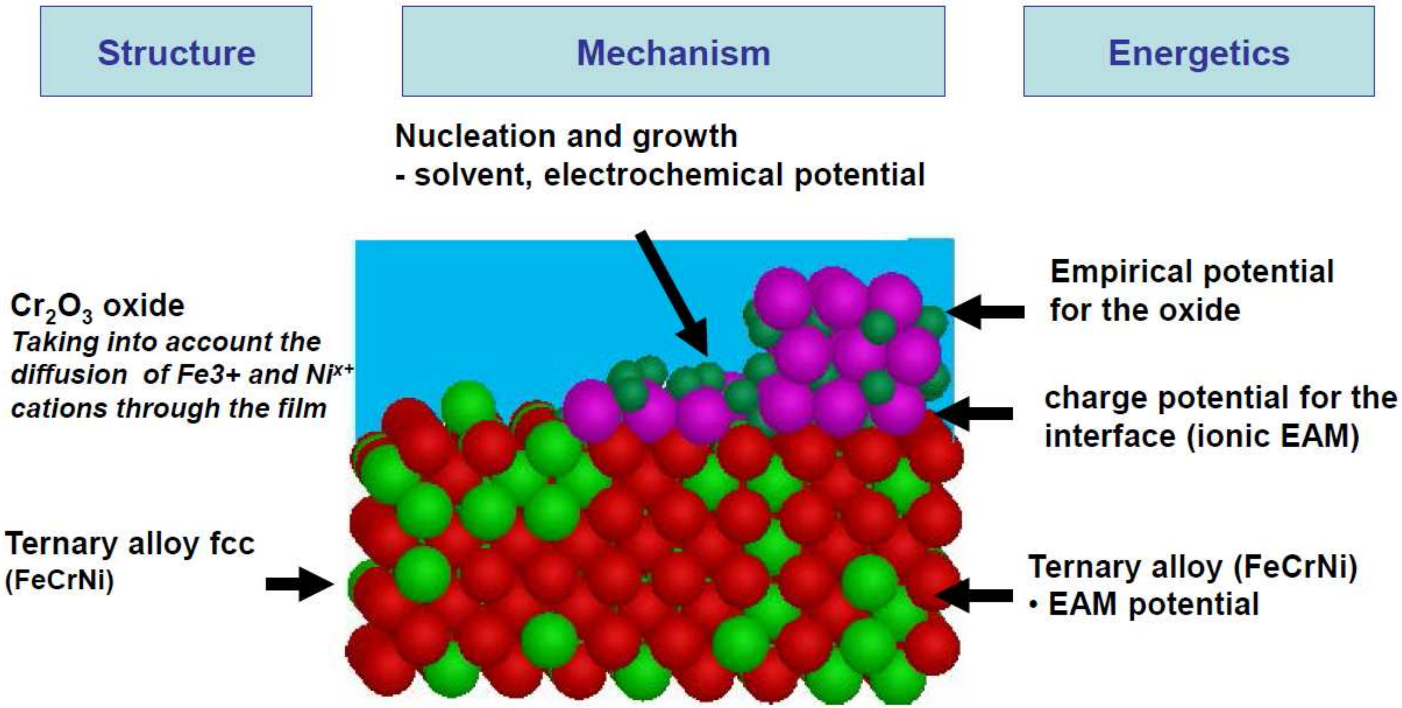


Figure 31: The main process of the VOL model approach to atomic-scale modelling of the metal oxide on a ternary Fe-Cr-Ni alloy (CNRS-LPCS).

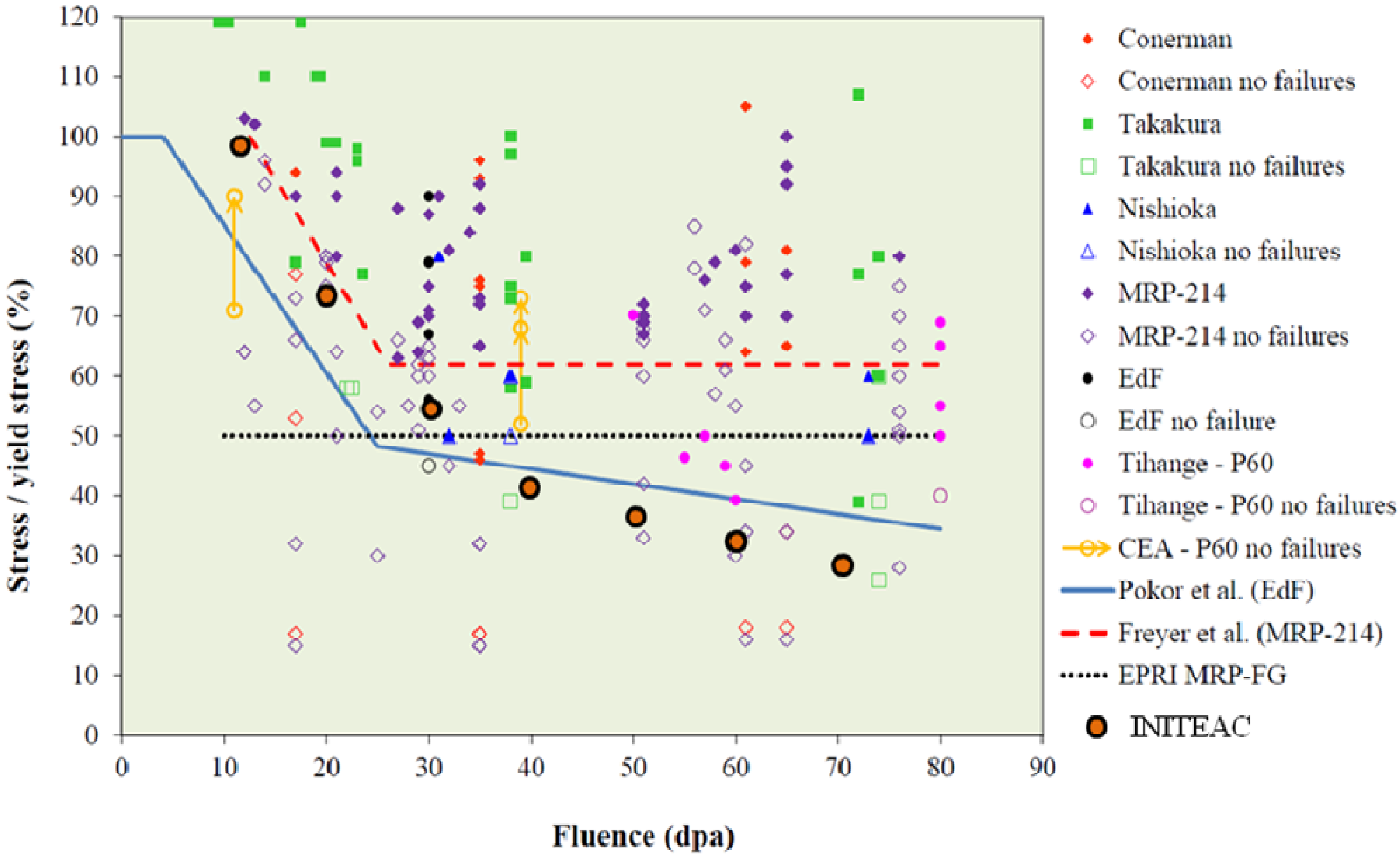


Figure 32: Experimental failure/non-failure threshold data together with INITEAC results

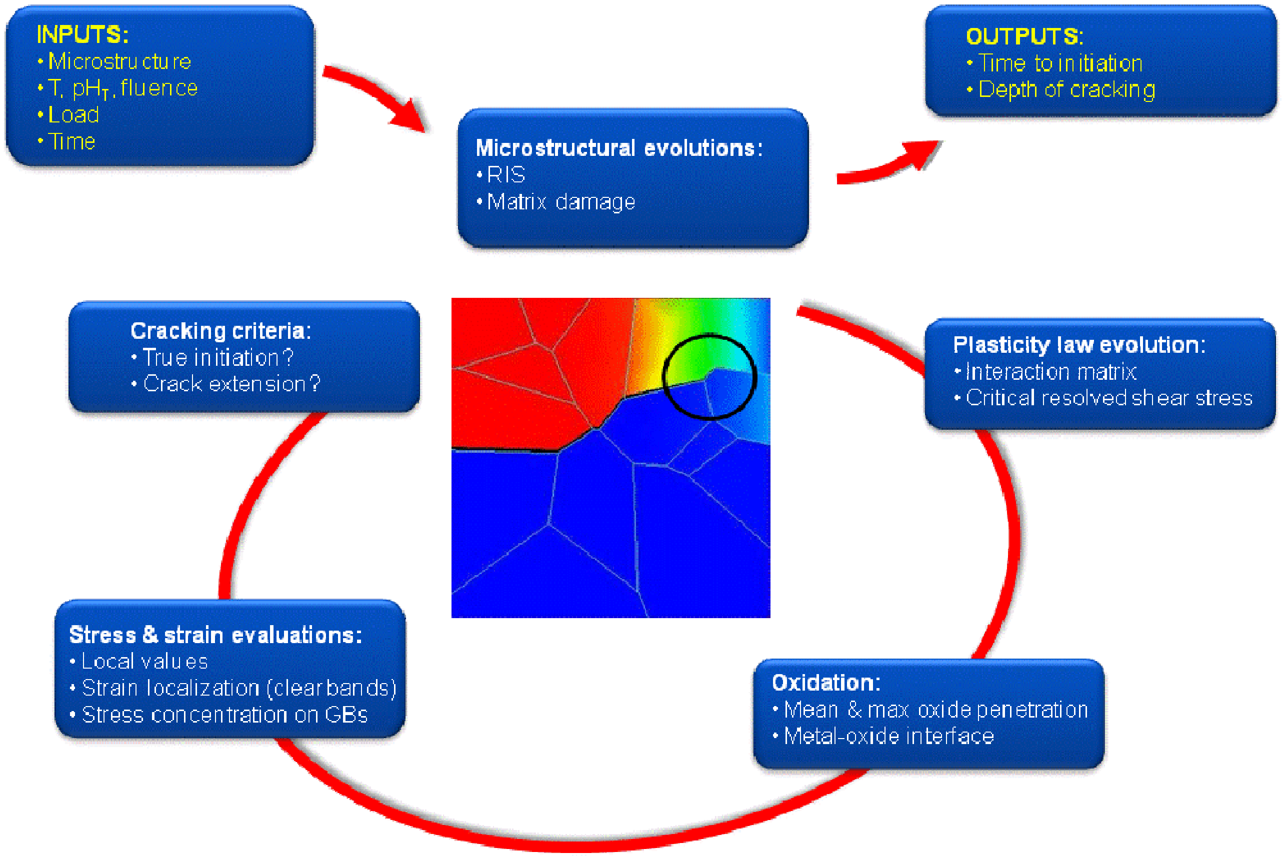


Figure 33: Scheme of coupling individual mechanisms in IGOC module

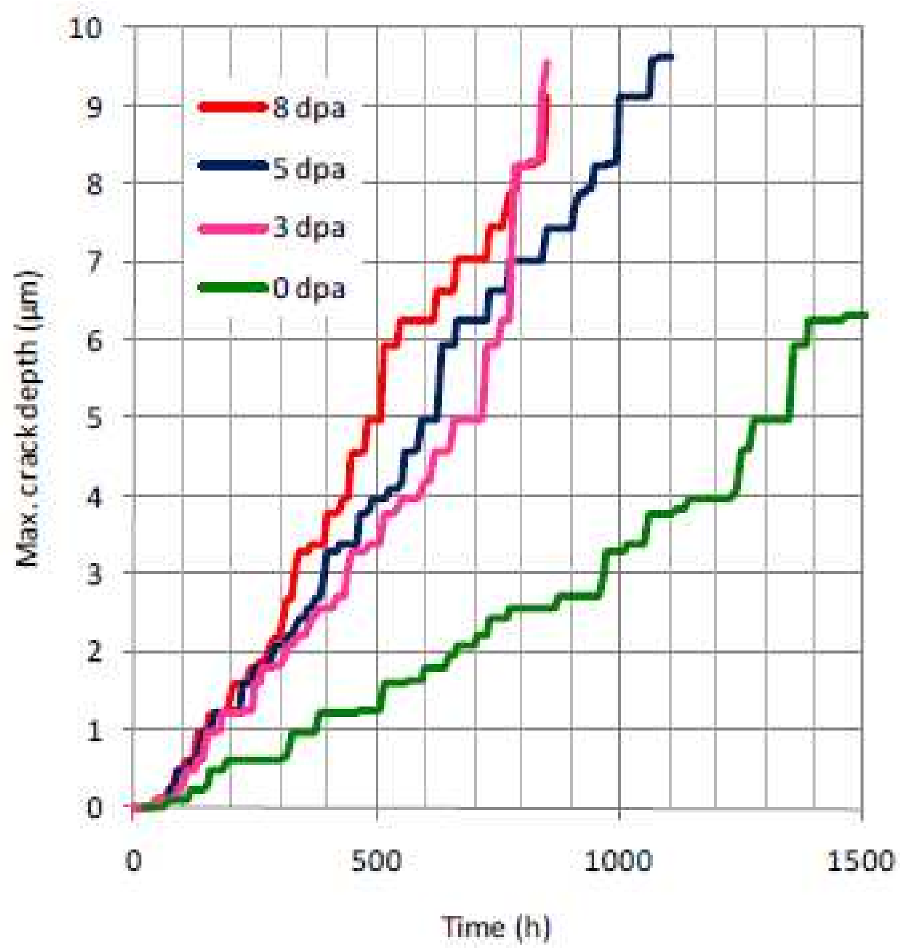


Figure 34: Example of IGOC simulation results

Figure 35: Table on the progress related to internals

PERFECT	**PERFORM60**
- Simulation of radiation damage in Ni; - Simulation of irradiation induced microstructure change in FeNi binary alloy ; - Long term simulation of irradiation induced defects in « green material » with (MFVISC) ; - Hardening mechanisms in pure Cu, and to some extend in FeNi (mostly interaction with loops and SFT's) ; - Simulation code to predict the local chemistry in crevices (T, pH, …) ; - Model for crack propagation ; - First version of a 2-D Monte carlo model for initiation; - No module was integrated in the platform PERFECT;	- Development Many versions (6) of FeNiCr ternary alloy potential; - Simulation of radiation damage in FeNi, FeNiCr ; - Microstructural evolution of radiation damage in FeNiCr (OKMC) - Long term simulation of radiation damage: development of CRESCENDO code; - Simulation of radiation induced segregation in FeNiCr and steels : development of 3 models (atomistic, analytic, and mean field) - Understanding the mechanisms of radiation induced hardening in FeNiCr (interaction of dislocations with various defect clusters) ; - Development of a physically based crystalline plasticity law for non and irradiated stainless steel and its experimental validation; - Prediction of stress-strain behavior of stainless steel under irradiation; - Simulation of the chemical environment as function of pH, T, …; - Model to predict the kinetics of corrosion with and without irradiation as function of materials properties (cold work, composition, …) temperature and environment chemistry; - Development of computational scheme to couple corrosion (slow process) and mechanical deformation (fast) during the same simulation; - Development of physical criteria governing the process of grain boundaries cracking - Development of statistical model for IASCC initiation (INITEAC) based on physical criteria (strain localisation, grain boundary decohesion, …) - Development of a deterministic model for crack initiation based on the integration of most of the above cited developments. - Experimentally: First experimental analysis of in-service failed bolt; IASCC initiation testing of highly active material (up to 80dpa) issued from an operating NPP, great amount of data related to the microstructural evolution, the corrosion behavior and mechanical properties of irradiated model alloys and steels (ion, proton, neutrons), - Development and production of the first simulation platform for IASCC initiation,

References

4.2 Use and dissemination of foreground

Section A (public)

Publications

LIST OF SCIENTIFIC PUBLICATIONS, STARTING WITH THE MOST IMPORTANT ONES											
No.	Title / DOI	Main author	Title of the periodical or the series	Number, date or frequency	Publisher	Place of publication	Date of publication	Relevant pages	Permanent identifiers (if applicable)	Is open access provided to this publication ?	Type
1	Sink strength calculations of dislocations and loops using OKMC http://dx.doi .org/10.1016/j.jnucmat.20 13 .08.052	V. Jansson , L. Malerba , A. De Backer , C.S. Becq uart , C. Domain	Journal of Nuclear Materi als	Vol. 442/I ssu e 1-3	Elsevier	Netherlands	01/11/2013	218-226			Peer revie wed
2	Comments on “Atomistic modeling of an Fe system with a small concentration of C” http://dx.doi .org/10.1016/j.commatsci. 20 13.09.048	R.G.A. Veiga , C.S. Becqu art , M. Perez	Computational Materials S cience	Vol. 82	Elsevier	Netherlands	01/02/2014	118-121			Peer revie wed
3	Orowan strengthening at low temperatures in bcc materials studied by dislocation dynamics simulations http://dx.doi .org/10.1016/j.actamat.20 10 .09.039	G. Monnet , S. Naamane , B. Devincre	Acta Materialia	Vol. 59/Is sue 2	Elsevier Limited	United Kingdom	01/01/2011	451-461			Peer revie wed
4	Low temperature deformation in iron stud ied with dislocation dynamics simulations http://dx.doi .org/10.1016/j.ijplas.200 9. 05.003	S. Naamane , G. Monnet , B. Devincre	International Journal of Plasticity	Vol. 26/Is sue 1	Elsevier Limited	United Kingdom	01/01/2010	84-92			Peer revie wed
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	http://dx.doi .org/10.1016/j.actamat.20 13 .07.023	M.-H. Chav anne , E. Ait , P. Francios i									
6	Transfer of molecular dynamics data to d islocation dynamics to assess dislocation–dislocation loop interaction in iron http://dx.doi .org/10.1016/j.scriptamat .2 013.06.026	D. Terentye v , G. Monnet , P. Grigorev	Scripta Materialia	Vol. 69/Is sue 8	Elsevier Limited	United Kingdom	01/10/2013	578-581			Peer revie wed
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8	Solute–point defect interactions in bcc systems: Focus on first principles model ling in W and RPV steels http://dx.doi .org/10.1016/j.cossms.201 2. 01.001	C.S. Becquart , C. Domain	Current Opinion in Solid State and Materials Science	Vol. 16/Is sue 3	Elsevier Limited	United Kingdom	01/06/2012	115-125			Peer revie wed
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11	Validating molecular dynamics with direct imaging of radiation damage debris 10.1103/PhysR evB.85.094111	P. D. Lane , G. J. Gallow ay , R. J. Cole , M. Caffio , R. Schaub , G. J. Ackland	Physical Review B - Conde nsed Matter and Materials Physics	Vol. 85/Is sue 9	American Physical So ciety	United States	01/03/2012	1-6			Peer revie wed
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64	Influence of plastic slip localization on gra in boundary stress fields and microcrack nucleation	M. Sauzay, ?K. Vor	Engineering Fracture Mech anics	110	Elsevier BV		01/01/2013	330-349			Peer revie wed
65	Clear band formation in irradiated FCC m etals: a 3 D dislocation dynamics invest igatio n	K. Gururaj, C. Robertso n, M. Fivel	Philosophical Magazine	tbc	Taylor and Francis L td.		01/01/2014	tbc			Peer revie wed
66	Determination of the critical resolved shear stress and the friction stress in austenitic	Monnet G.? Pouchon M.	Materials Letters	98	Elsevier		01/01/2013	128-130			Peer revie wed

	stainless steels by compression of pillars ex tracted from single grains										
67	Characterizat ion of SEM speckle pattern marking and imaging distorsion by Digital Image Correlation	Adrien Gué ry?Félix L atourte ?Fr ançois Hild and Stéphane Roux	Measurement Science and Technology	tbc	Institute of Physics Publishing		01/01/2014	tbc			Peer revie wed
68	Towards a modelling of RPV steel brittle fracture using crystal plasticity computatio ns on polycrystalli ne aggregates	L. Vincent et al.	Journal of Nuclear Materi als	406	Elsevier		01/01/2010	91			Peer revie wed
	Orowan Strengthening and forest hardenin g superposition examined by dislocation dynamics simulations	Queyreau S .Monnet G. Devinc re B.	Acta Materiala	58			01/01/2010	5586		No	Article
	Iron-Copper-N ickel Many-Body Potential Consistent with Thermodynami cs	Bonny G., Pasianot R., Castin N., T erentye v D., Malerba L.	Proceedings of the 17th I nternationa l Conference on Nuclear Engineering		ASME New York, NY, United States	USA	15/07/2009				Conference
	Many-body interatomic potentials to model radiation damage in reactor pressure vessel steels and in-core components	Bonny G., Pasianot R., Malerba L.	Of the 2nd International Youth Conference on Energetics		Budapest University of Economics and Tec hnology	Budapest	05/06/2009				Conference
	Positron defect studies of neutron irradiated iron-based materials	Lambrecht M., Al Maz ouzi A.	17th Internationa l Confer ence on Nuclear Engineeri ng		ASME	NY	14/07/2009	297 - 305			Conference
	The influence of irradiation-i nduced mic rostructur e on the hardening of RPV steels	Lambrecht M., Al Maz ouzi A.	ICONE 17		ASME	NY	15/07/2009	289- 293			Conference

LIST OF DISSEMINATION ACTIVITIES								
No.	Type of activities	Main Leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
1	Organisation of Workshops	ELECTRICITE DE FRANCE S.A.	international worksh op on multi-scale si mulation of the pred iction of radiation damage in reactor pr essure vessel steels and internals up to 60 years of operati on	10/12/2013	EDF Lab. Les Re nardières, 77818 Moret sur Loing Fr ance	Scientific comm unity (higher educat ion, Research) - Ind ustry	116	France, blgium, Germany, Switz erland, Finland, UK, Sweden, C zeck republick, USA, Japan, Russia
2	Organisation of Conference	ELECTRICITE DE FRANCE S.A.	International group of radiation damage in materials	20/05/2013	Embiez Island, France	Scientific comm unity (higher educat ion, Research) - Ind ustry	120	Fr, B, D, Fi, S, CH, UK, USA, J, Ru, Ho, Bu, Cz, China, Bu, Ho, Ro,
3	Oral presentation to a scientific event	Serco Limited	In-Situ Optical Stud ies of Stress Corros ion Crack Initiation in 304 Stainless St eel in High Tem peratures Oxyge nated Water	20/04/2010	Risley, UK	Scientific comm unity (higher educat ion, Research)		International
4	Oral presentation to a scientific event	Rolls-Royce Power Engineering PLC	The Perform 60 Users' Group : an in vitation to join	12/10/2009	Budapest	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	international
5	Oral presentation to a scientific event	TRACTEBEL ENGINEERING S.A.	IASCC Meeting	21/10/2009	Palo Alto	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
6	Oral presentation to a scientific event	STUDIECENT RUM VOOR K ERNENERGIE	94 th national meeti ng of the Argentine Physics Association	18/09/2009	Rosario	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
7	Oral presentation to a scientific event	STUDIECENT RUM VOOR K ERNENERGIE	Characterisation of defects in Fec syste ms	18/10/2009	Rochehaut sur S emois Belgique	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
8	Oral presentation to	STUDIECENT	KarakTerisering av	13/11/2009	Helsinki	Scientific comm	100	International

	a scientific event	RUM VOOR K ERNENERGIE	defekter I Fec-S ystem			unity (higher educat ion, Research) - Ind ustry		
9	Oral presentation to a scientific event	STUDIECENT RUM VOOR K ERNENERGIE	2nd International Yo uth Conference on Energetics	05/06/2009	Budapest	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
10	Oral presentation to a scientific event	STUDIECENT RUM VOOR K ERNENERGIE	Iron-Copper-Nickel Many Body Potent ial Consistent with Thermodynamics	16/07/2009	Brussels	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
11	Oral presentation to a scientific event	ELECTRICITE DE FRANCE S.A.	17th International C onference on Nu clear Engineering	12/07/2009	Bruxelles	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
12	Oral presentation to a scientific event	ELECTRICITE DE FRANCE S.A.	Positron Defect stud ies of neutron irrad iated iron-based mat erials	16/07/2009	Bruxelles	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
13	Oral presentation to a scientific event	THE UNIVERSITY OF MANCHESTER	IGRDM 15	11/10/2009	Budapest	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
14	Oral presentation to a scientific event	UNIVERSITAT POLITECNICA DE CATALUNYA	Interaction of carbon atoms with self in sterstitial atom clu sters & dislocations in a-Fe	12/09/2011	Montpellier, France	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
15	Oral presentation to a scientific event	STUDIECENT RUM VOOR K ERNENERGIE	Calculation of prope r vacancy migration energy barriers with artificial neural n etworks for the modelling of vacanc y clusters' migration	15/07/2010	Krakow, Poland	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
16	Oral presentation to a scientific event	STUDIECENT RUM VOOR K ERNENERGIE	Interaction of carbon with point defect clusters in alpha-ir on: An MD study	15/07/2010	Krakow, Poland	Scientific comm unity (higher educat ion, Research) - Ind ustry	100	International
17	Oral presentation to a scientific event	COMMISSARIAT ENERGIE ATOM	Irradiation Induced solute segregation in	06/06/2010	Avignon, France	Scientific comm unity (higher educat	100	International

		IQUE CEA	an under saturated Fe-1% at Mn ferritic model alloy			ion, Research) - Industry		
18	Oral presentation to a scientific event	COMMISSARIAT ENERGIE ATOMIQUE CEA	Late-Blooming Phase Investigation in an Ion Irradiated Fe-1wt.%Mn alloy	16/02/2010	San Diego, USA	Scientific community (higher education, Research) - Industry	100	International
19	Oral presentation to a scientific event	ELECTRICITE DE FRANCE S.A.	Identification of lattice friction in coherent precipitates from atomistic to continuum scale	15/10/2012	Singapore	Scientific community (higher education, Research) - Industry	100	International
20	Oral presentation to a scientific event	UNIVERSITAT POLITECNICA DE CATALUNYA	Slip system activity in Fe and Fe-C alloys	15/08/2012	Budapest	Scientific community (higher education, Research) - Industry	100	International
21	Oral presentation to a scientific event	ELECTRICITE DE FRANCE S.A.	Dislocation Dynamics based crystalline law for low temperature plastic deformation of iron	15/10/2010	San Diego, USA	Scientific community (higher education, Research) - Industry	100	International
22	Oral presentation to a scientific event	ELECTRICITE DE FRANCE S.A.	Stochastic analysis of thermally activated dislocation processes simulated by molecular dynamics	15/10/2010	Freibourg, Germany	Scientific community (higher education, Research) - Industry	100	International
23	Oral presentation to a scientific event	ELECTRICITE DE FRANCE S.A.	Dislocation nucleation from free surfaces in iron : surface resistance to local shear stresses	15/05/2010	Paris, France	Scientific community (higher education, Research) - Industry	100	International
24	Oral presentation to a scientific event	ELECTRICITE DE FRANCE S.A.	Modeling and Dislocation Dynamics Study of the Orowan Mechanism	15/02/2009	San Francisco, USA	Scientific community (higher education, Research) - Industry	100	International
25	Oral presentation to a scientific event	ELECTRICITE DE FRANCE S.A.	MS Simulations of edge dislocation nucleation from free surfaces in iron	15/09/2009	Barcelona, Spain	Scientific community (higher education, Research) - Industry	100	International
26	Oral presentation to a scientific event	ELECTRICITE DE FRANCE S.A.	Multiscale Simulations How can dislocati	11/09/2009	Lisbon	Scientific community (higher educat	100	International

			on Dynamics Simulations Account for Atomic Simulation Results			ion, Research) - Industry		
27	Oral presentation to a scientific event	COMMISSARIAT ENERGIE ATOMIQUE CEA	Application of Microstructure Informed Brittle Fracture model to the cleavage of an RPV steel	20/05/2013	Toulon, France	Scientific community (higher education, Research) - Industry	100	International
28	Oral presentation to a scientific event	COMMISSARIAT ENERGIE ATOMIQUE CEA	Fracture Modelling	15/06/2012	Brescia	Scientific community (higher education, Research) - Industry	100	International
29	Oral presentation to a scientific event	COMMISSARIAT ENERGIE ATOMIQUE CEA	Micromécanique de la rupture	15/07/2012	Brno	Scientific community (higher education, Research) - Industry	100	International
30	Oral presentation to a scientific event	COMMISSARIAT ENERGIE ATOMIQUE CEA	Symposium Sir Cottrell	15/06/2013	Pekin	Scientific community (higher education, Research) - Industry	100	International
31	Oral presentation to a scientific event	COMMISSARIAT ENERGIE ATOMIQUE CEA	Confernce Material at Extremes	11/07/2013	New England	Scientific community (higher education, Research) - Industry	100	International
32	Oral presentation to a scientific event	COMMISSARIAT ENERGIE ATOMIQUE CEA	The irradiation assisted Stress Corrosion Cracking (IASCC)	05/12/2012	Paris, France	Scientific community (higher education, Research) - Industry	100	International
33	Oral presentation to a scientific event	COMMISSARIAT ENERGIE ATOMIQUE CEA	Dislocation and Irradiation Defects-Based Micromechanical	08/01/2013	Paris	Scientific community (higher education, Research) - Industry	100	International
34	Oral presentation to a scientific event	VALTION TEKNILLINEN TUTKIMUSKESKUS	Deformation microstructures of 30 dpa AISI 304 stainless steel after monotonic tensile & constant load autoclave testing	07/08/2011	TMS	Scientific community (higher education, Research) - Industry	100	International
35	Oral presentation to	COMMISSARIAT	Influence of slip lo	28/06/2010	Brno, Republique	Scientific comm	100	International

	a scientific event	ENERGIE ATOMIQUE CEA	calization on surface relief formation and grain boundary microcrack nucleation		Tcheque	unity (higher education, Research) - Industry		
36	Oral presentation to a scientific event	ELECTRICITE DE FRANCE S.A.	Simulation de la réponse mécanique d'un acier inoxydable austénitique à l'aide de calculs cristallins	09/05/2011	Giens, France	Scientific community (higher education, Research) - Industry	100	International