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Towards a single European strategic research and innovation agenda on materials for all reactor generations through dedicated projects

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Abstract. The goal of the ORIENT-NM action is to produce a single European strategic vision on research and innovation concerning nuclear materials in the EU, serving all reactor generations and nuclear systems. The key in this endeavour is to focus on advanced materials science practices that, combined with digital techniques, will enable acceleration in materials development, manufacturing, supply, qualification, and monitoring, in support of nuclear energy safety, efficiency, economy and sustainability. The research agenda will be rooted in existing virtuous examples of nuclear materials science projects. Here the results of three of them are summarised, thereby covering different reactor applications and families of materials, as well as a range of advanced material research approaches. GEMMA addressed a number of key areas concerning the development and qualification of metallic structural materials for GenIV reactor conditions, focusing on austenitic steels and their compatibility with several non-aqueous coolants, their welds and the modelling of their stability under irradiation. INSPYRE was an integrated project applying a basic science approach to $(U,Pu)O_2$ fuels, to develop physics-based models for the behaviour of nuclear fuels under irradiation and improve fuel performance codes. Modelling was also the focus of the M4F project, which brought together the fission and fusion materials communities to study the effects of localised deformation under irradiation in ferritic/martensitic steels and to develop good practices to use ion irradiation as a tool to evaluate radiation effects on materials.

1 Introduction

The ORIENT-NM project is elaborating a single European strategic research and innovation agenda (SRIA) that should set the path for future activities on nuclear materials in the EU until 2040, serving all reactor generations. The key in this endeavour is to focus on advanced materials science practices that, combined with modern digital techniques, will enable acceleration in materials development, manufacturing, supply, qualification, and monitoring, in support of nuclear energy safety, efficiency, economy and sustainability. This research agenda, which pursues five transversal research lines, is rooted in existing virtuous examples of materials science projects that target nuclear energy innovation. The objectives and key results of three of them, which cover different reactor applications and families of materials, are presented in this paper, illustrating the advances brought by the various research lines considered in ORIENT-NM. GEMMA addresses a number of key areas concerning the development and qualification of metallic structural materials for Gen IV reactor conditions: (1) corrosion-resistance of austenitic steels for application in heavy-liquid metal-cooled systems; (2) production of welds of available austenitic steels and their characterization in terms of internal stresses; (3) testing of these materials (baseline, welds and advanced) under representative conditions in contact with heavy liquid metals and helium; (4) development of physical models for the prediction of the behaviour of austenitic alloys under long term irradiation. The INSPYRE project applied a basic science approach to $(U,Pu)O_2$ fuels to get further insight into the mechanisms underlying their changes under irradiation, and accordingly develop physics-based models that describe the behaviour of nuclear fuels under irradiation and improve European fuel performance codes. Finally, the M4F project created a bridge between fission and fusion materials communities by applying physical modelling techniques to target two objectives: (1) understand and predict the origin and effects of localised deformation under irradiation in ferritic/martensitic steels,

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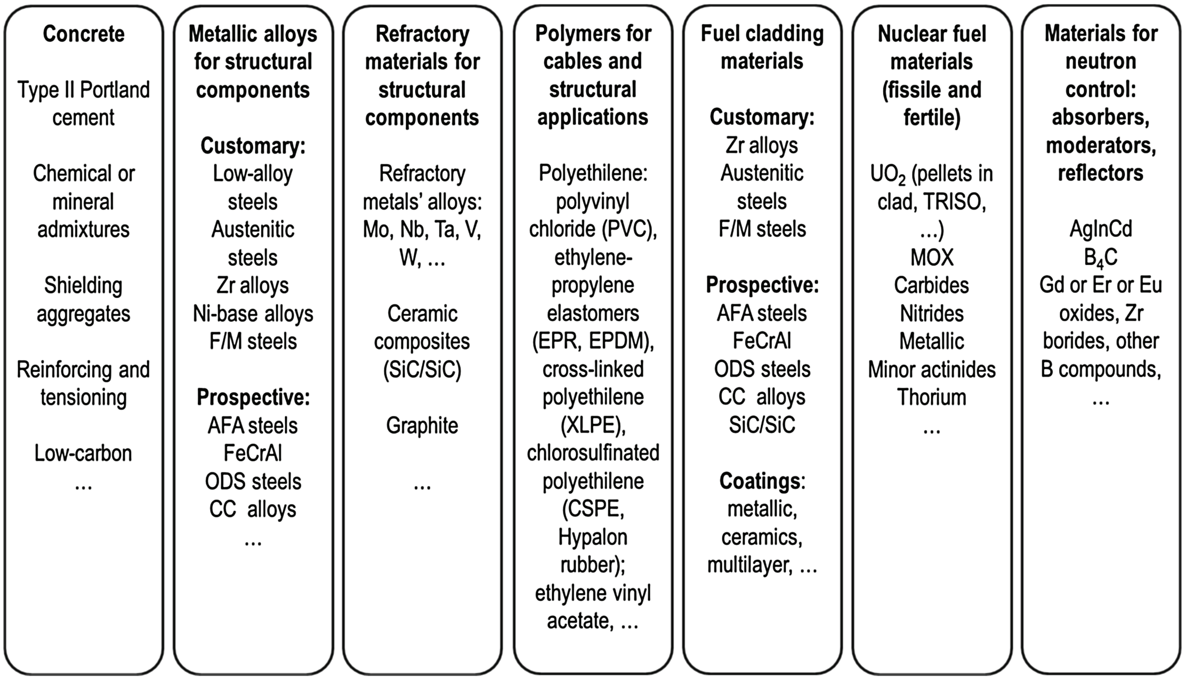

Fig. 1. Classes of nuclear materials and their variety.

which affect the mechanical behaviour of components for future fission and fusion reactors, to enable their design based on robust standards; (2) to develop good practices to use ion irradiation as a tool for the evaluation of radiation effects on materials, also applied to ferritic-martensitic alloys. The objectives and structures of these projects are described in [1]. All the projects described in this article are part of the activities of the Joint Programme on Nuclear Materials of the European Energy Research Alliance [2].

2 ORIENT-NM: a single vision on nuclear materials research for all reactor generations until 2040

ORIENT-NM (Organisation of the European Research Community on Nuclear Materials) is a Coordination and Support Action (CSA) partially funded by the Euratom research and training work programme 2019–2020. It was launched to explore the opportunity of setting up a European partnership on nuclear materials, establishing the relevant Strategic Research Agenda (SRA) and governing structure, while defining its interactions with external stakeholders. The starting point for this was the analysis of the national energy and climate plans (NECP) [3], as well as other documents that are available online, such as the IAEA and WNA country nuclear power profiles [4,5]. This enabled the different national priorities to be identified, in connection with nuclear energy and materials in the EU member states. This analysis [6] revealed, among other things, that a significant number of EU member states intend to maintain or even expand their nuclear-installed power through long-term operation (LTO), power uprates and new builds, from now to 2040. In addition, game-changers such as small modular reactors and advanced designs of interest throughout the continent may lead nuclear energy to be even more widespread in 2040 than currently foreseeable. Recent dramatic geopolitical events might also have an impact on this.

In this framework, materials research plays a crucial role to enhance the safety, efficiency, economy, and overall sustainability of current reactors and enabling the commissioning and deployment of next-generation reactors, as well as fusion. The nuclear materials science community in Europe is therefore called to provide the tools, knowledge and skills to enable each European country to maintain the wished and needed nuclear capacity and/or, depending on national policies and interests, to develop advanced nuclear systems, within the time horizon of 2040. Specifically, it should contribute to enabling EU member states to:

- ensure safe and affordable LTO of current generation reactors;
- design, license and construct Gen III+ new builds over the next two decades;
- deploy light water SMRs within the next decade;
- facilitate and reduce the time and costs for design, licensing, and construction of competitive next-generation nuclear reactors, including advanced SMRs, within the 2040 horizon.

The materials involved a priori range from concrete and metallic structural alloys, to polymers, fuel and compounds for neutron control, as is shown in Figure 1. In order to enable progress towards enhanced safety, efficiency and economy, the development, manufacturing and qualification of innovative materials must be accelerated,

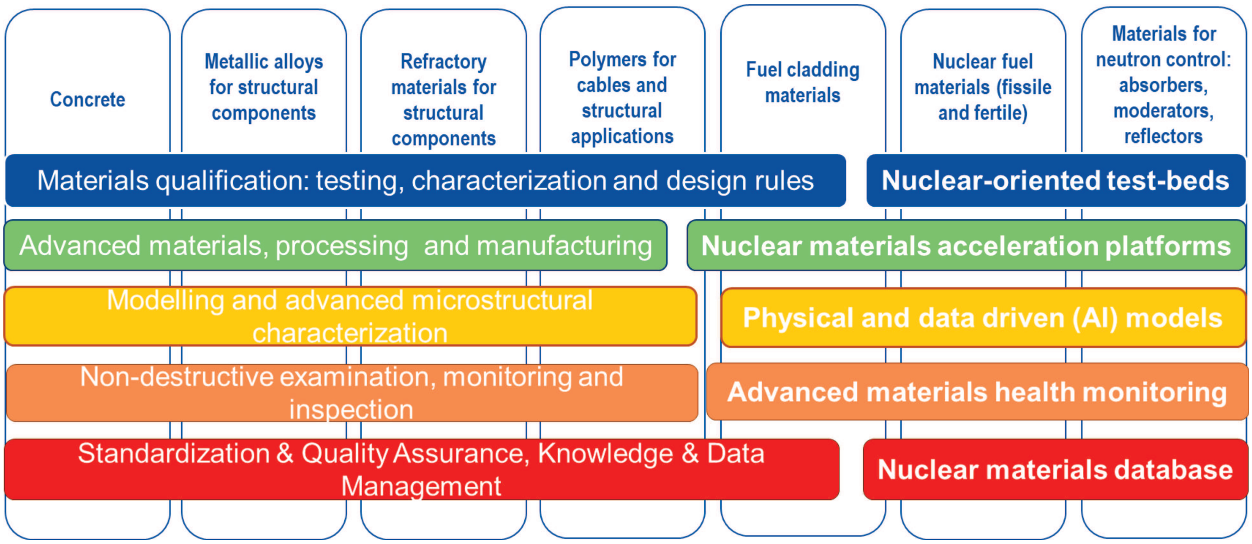

Fig. 2. The five transversal research lines and Grand Goals proposed in ORIENT-NM.

thus reducing their time to market. Accurate health monitoring while operating is also needed. This implies a shift from the traditional "observe and qualify" to the modern "design and control" materials science approach. Advanced digital techniques and suitable models are the enablers of this shift.

Five materials science practices and relevant research lines constitute accordingly the Grand Goals to be pursued within the next decade:

(a) establishment of an integrated European system for the efficient application of advanced and suitably standardized experimental procedures and methodologies for nuclear materials characterization, testing and qualification, be they destructive, non-destructive or microstructural; i.e., nuclear test-beds;
(b) development of methodologies for accelerated, targeted and systematic nuclear materials improvement, or even discovery, including the whole range of variables of relevance; i.e., nuclear materials acceleration platforms (MAPs), which promise to be key to reducing the time to market of innovation;
(c) development of combined physical and data-driven models and predictive methodologies of direct application for industrial needs;
(d) development of advanced methods for materials and component health monitoring through non-destructive examination and testing, coupled with diagnostics and simulation tools, to enable the implementation of digital twins;
(e) establishment and use of efficient platforms and procedures for data collection, storage and management (European nuclear materials FAIR[1] database).

Nuclear test beds and MAPs inherently require coordinated use of (present and future) European facilities and infrastructures and exploitation of available schemes and roadmaps for access to and use of major infrastructures (chiefly materials testing reactors and ion irradiation facilities, but also facilities for the exposure to fluids and the subsequent characterization). The transversal nature of the above five research lines and Grand Goals is illustrated in Figure 2. The first corresponding proposal of the Strategic Research Agenda has been published in [7].

3 GEMMA: qualification of austenitic steels for application in GenIV prototypes and demonstrators

The GEMMA project (GenIV Materials Maturity), which ended in November 2021, was partially funded by the Euratom research and training work programme 2014–2018. It mainly addressed the following areas: (1) production and characterization of advanced alumina forming corrosion-resistant austenitic steels for application in heavy-liquid metal-cooled systems; (2) characterization of welds on available austenitic steels in terms of internal stresses; (3) testing under representative conditions in contact with heavy liquid metals and helium; (4) development of physical models for the prediction of the behaviour of austenitic alloys under long term irradiation. The results on these topics are summarised below.

3.1 Advanced alumina forming corrosion-resistant austenitic steels for application in heavy-liquid metal-cooled systems

Alumina-forming austenitic stainless steels (AFA) and Al-based diffusion coatings are candidates for application in heavy liquid metals at high temperatures, to replace conventional stainless steels, which exhibit poor performance in these environments [8]. In the GEMMA Project, more than 20 AFA model alloys were produced by the industrial partner SANDVIK and compared.

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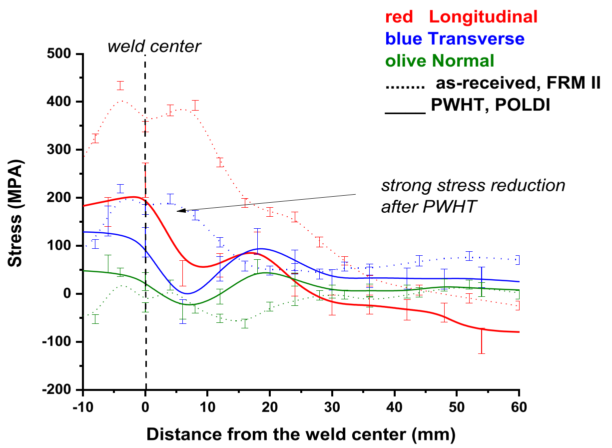

Fig. 3. Diffractometric measurements of internal stresses, before and after PWHT.

They were all exposed to liquid Pb under various conditions. Selected AFA alloys were also exposed to steam at 1200 °C to explore their potential use in a steam environment. Their microstructure was then analysed to investigate their corrosion resistance. The AFA model alloys with the composition formulas Fe–(15.2–16.6)Cr–(3.8–4.3)Al–(22.9–28.5)Ni (wt.%) and Fe–16Cr–(23–25.5)Ni–(3–4.5)Al–C(N)–(Y) have all shown corrosion resistance to oxygen-containing molten Pb at 600 °C. By increasing the exposure temperature to 650 °C, only the alloy of the first family, with the lower Ni content (∼23 wt.%), and with minor additions of Nb and Y, forms a protective oxide scale. Higher Ni contents increase the susceptibility to corrosion attack at 650 °C in Pb. The passivating scale was based on $(AlCr)_2O_3$ at both temperatures and formed a homogeneously alloyed coating with the expected composition. To evaluate the microstructural stability of AFA alloys at elevated temperatures, thermal ageing experiments were performed at 600 °C for 1000 and 2000 h and 650 °C for 3550 h. The austenitic phase was preserved, but all the alloys exhibited secondary phases and precipitations [9].

3.2 Characterization of welds on available austenitic steels in terms of internal stresses

High-resolution neutron diffraction residual stress measurements on a welded coupon after Post-Weld Heat Treatment (PWHT) were carried out at the spallation neutron source SINQ in Villigen (CH). An identical coupon had been studied by high-resolution neutron diffraction stress measurements in the as-welded state at FRM-II in Garching. The PWHT consisted of a dwelling temperature of 700 °C for 24 h with limited heating and cooling rates: these relatively high temperatures and long dwelling time were chosen to ensure tangible relaxation of residual stresses, but bore no connection with the heat treatment process prescribed by the RCC-MRx code. Diffractometric measurements were carried out on both coupons at the POLDI instrument (Pulsed Over-Lap DIffractometer). Figure 3 shows that the PWHT was effective to reduce the stresses inside the weld and the heat-affected zone, as well as to reduce the width of the stress gradient, particularly in the longitudinal direction. The maximum stress values are more than halved and stress lower than 100 MPa are found already at a 10 mm distance from the weld centre.

3.3 Testing under representative conditions in contact with heavy liquid metals and helium

An extensive experimental campaign was carried out to obtain data on the compatibility of base materials (austenitic alloys 316L and 15-15Ti), their welds, AFA, and coated specimens (alumina forming diffusion coatings, ceramic coatings by pulsed laser deposition and by detonation gun spray) with heavy liquid metals (HLM) and He gas. The goal was to clarify the degradation mechanisms and to establish correlations for the design of MYRRHA [10], ALFRED [11] and ALLEGRO [12]. For the first time, a large amount of data has been collected on the compatibility of steels and their welds in contact with these fluids. Thermodynamic simulations with the CALPHAD method and with atomistic modelling have supported the experimental work, to gather information on the relevant part of the phase diagrams of the complex oxide systems and the mass transport properties of the compounds that form.

Contrary to common perception, the corrosion in molten lead and lead-bismuth eutectic (LBE) differed both for the severity of the attack and the mechanisms, the dissolutive attack in LBE being more severe. Furthermore, while the lead dissolving process mainly concerns nickel, in LBE both chromium and nickel are dissolved. In particular, the corrosion campaign in flowing Pb in the testing loop MATLOO at CV-Rez showed that, after 16 000 to 18 000 h at 480 °C, with oxygen concentration 10^{-7} wt.% and 1.6 m/s flow velocity, corrosion was negligible in all the exposed materials [13]. The ENEA corrosion campaign, carried out in the BID1 facility, in liquid Pb at 550 °C with low oxygen concentration (10^{-8}–$10^{-7\%}$ wt.%) up to 8000 h, led to the interesting observation that the magnitude of the corrosion of welds in terms of the depth of penetration was low compared to the corrosion observed in base materials under the same conditions. The microstructural investigations have not unambiguously clarified the relevant mechanisms, but the results suggest precipitation of the δ ferrite at grain boundaries and triple joints, which limits or prevents the rapid diffusion of nickel there. Moreover, pulsed-laser deposited alumina coatings confirmed their superior protective action on 15-15Ti, while both selected AFA alloys showed low yearly corrosion [14,15].

Opposite results were obtained in tests in LBE, with the poorer performance of welded joints versus the base material. The unacceptable corrosive attack on welded joints calls for additional measures for their protection in LBE. Investigations aimed at studying the corrosion mechanisms highlighted that the initiating process of the attack in HLM is the dissolution of iron from the

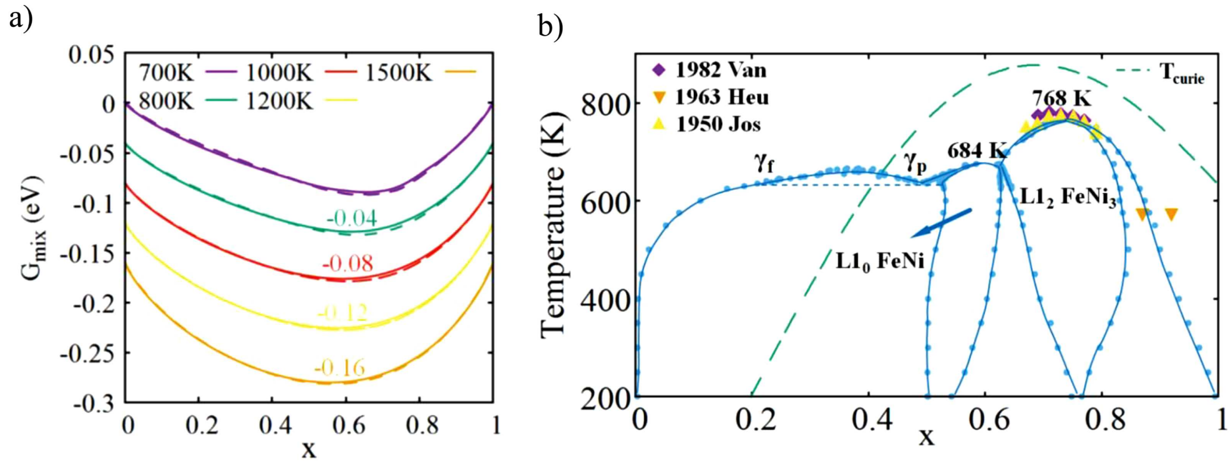

Fig. 4. (a) Gibbs free energy of mixing of the Fe–Ni solid solution of the pair interaction model (full lines) and CALPHAD (dotted lines), at different temperatures. For the sake of clarity, each curve (except at 700 K) is shifted downwards by the value given in the figure. (b) the Fe–Ni FCC phase diagram: comparison between the pair interaction model and experiments.

native iron-chromium oxide that protects the stainless steel in many environments. This dissolution leads then to the formation of a porous structure with interconnected channels along the grain boundaries, which is permeable to oxygen and the components of the steel. The inner Fe-Cr oxide provides channels for oxygen entering and iron leaching. Investigations have also shown that the subsequently formed layer of magnetite in turn loses its protective capability, due to the onset of wetting processes of the grain boundaries by the liquid metal, above temperatures around 450 °C. These results set limits on the applicability of oxygen control for corrosion control of HLM; on the other hand, they set a limit below which steels can be used safely in lead [14,16].

Finally, the mechanical testing campaign in HLM confirmed the absence of liquid metal embrittlement in the austenitic steels 316L and 15-15Ti. Yet, the intensity of the corrosion processes strongly depends on the microstructure of the steel. The presence of extended defects with negligible effects on the mechanical properties in the air could lead to deep corrosive attacks in HLM, with mechanical degradation that is solely linked to the reduction of the resistant section [17].

3.4 Development of physical models for the prediction of the behaviour of austenitic alloys under long-term irradiation

In the temperature range of interest for operation (300–700 °C), irradiation produces in austenitic alloys new microstructural features, such as new families of precipitates, solute segregations at structural defects, point defect clusters and voids, leading to dimensional changes (swelling) and worsening the mechanical properties (loss of ductility, hardening). These microstructural features induce adverse effects and limit the lifetime of the materials. Predictive models for microstructure evolution under irradiation are therefore useful tools in support of assessing the component lifetime. With this aim in mind, as the first step kinetic models were developed to describe the phase diagrams of Fe–Ni–Cr model alloys, their diffusion properties and the kinetics of segregation and ordering. The composition range of the ternary model alloy has been chosen to encompass those of 316L(N) and AIM1 steels, targeting temperatures around 500 °C. Interdiffusion experiments in Fe–Ni–Cr multi-layers during isothermal annealing and under ion irradiation have been performed to assess the validity of the atomistic kinetic models. Two thermodynamic descriptions were developed, one based on an implicit treatment of magnetism and a second one explicitly treating the magnetic interactions between Fe and Ni atoms. Relying on the former, a rigid lattice pair interaction diffusion model was developed and used for Atomic Kinetic Monte Carlo (AKMC) simulations in binary Fe–Ni alloys. The pair interactions were fitted to 0 K ab initio calculations of formation enthalpies of ordered and disordered structures and also systematically fitted on the Gibbs free energy of the γ Fe–Ni solid solution, as described in a CALPHAD (CALculation of PHAse Diagrams) study [18]. The model reproduces well the data for the solid solution (Fig. 4a) and the $FeNi_3$–$L1_2$ ordered phase in a large domain of composition and temperature, using first and second neighbour pair interactions which depend on temperature and local Ni concentration. The FCC phase diagram of the Fe–Ni system was determined using Monte Carlo simulations in the semi-grand canonical ensemble (Fig. 4) and compared with experimental studies and other models. In addition to the γ solid solution and the $FeNi_3$–$L1_2$ phase, the FeNi–$L1_0$ phase is found to be stable below 684 K. The model also predicts a phase separation between ferromagnetic (γf) and paramagnetic (γp) solid solutions.

The pair interaction model was then extended to include vacancy diffusion. Vacancy-pair and saddle-point interactions were fitted on electronic structure calculations of vacancy formation and migration energy and to experimental tracer diffusion coefficients in dilute alloys. AKMC simulations were performed to calculate tracer and interdiffusion coefficients in concentrated solid solutions and compared with available data. Finally, a BCC and FCC Fe–Ni phase diagram below the magnetic-transition temperatures based only on electronic structure calculation results was constructed. The free energy of the various phases was determined by including the vibrational and the ideal configurational entropies. The resulting phase diagram is in very good agreement with the experimental data and suggests possible improvements for upper-scale semi-empirical approaches (such as CALPHAD). In order to go further in the thermodynamic prediction of the Fe–Ni alloys at higher temperatures, when magnetic excitations and transitions occur, an effective interaction model for Fe–Ni, which describes chemical and magnetic interactions explicitly and the effect of vibrational entropy, was explored. This model is currently extended to describe the properties of defects (vacancies and self-interstitial atoms) in Fe–Ni for various chemical and magnetic states [19].

4 INSPYRE: basic research on U–Pu mixed oxide fuels to improve fuel performance codes

The INSPYRE project (Investigations Supporting MOX Fuel Licensing in ESNII Prototype Reactors), which ended in February 2022, was partially funded by the Euratom research and training work programme 2014–2018. INSPYRE aimed at:

(1) using a basic research approach that combines out-of-pile separate effect experiments with physical modelling and simulation to get further insight into the underlying phenomena that govern the behaviour of (U, Pu)O_2 mixed oxide (MOX) fuels under irradiation.
(2) Performing additional post-irradiation examinations (PIE) on selected samples to complete the results available in the literature.
(3) Extending the reliability regime of empirical laws that describe nuclear fuel under irradiation using the results obtained in the project, as well as those of previous integral neutron irradiation tests.
(4) Using these results to improve the reliability of European operational fuel performance codes in normal and off-normal situations to facilitate nuclear fuel licensing and improve safety.
(5) Training the next generation of researchers on nuclear fuels.

These objectives are presented in the project's video [20]. The results of the project are synthesised in [21] and summarised below.

4.1 Advances in the understanding and description of the behaviour of nuclear fuels

INSPYRE brought significant advances in the understanding of mechanisms that are crucial for the safety assessment and qualification of MOX fuels for future nuclear reactors, as well as in the simulation of the fuel behaviour in the reactor. The new experimental and modelling results significantly enhance the knowledge and understanding of the physical, thermal, chemical and mechanical properties of MOX fuels. In addition, several setups were developed to enable the detailed characterization of UO_2 and plutonium- and americium-bearing fuels in the hot laboratories of the partners.

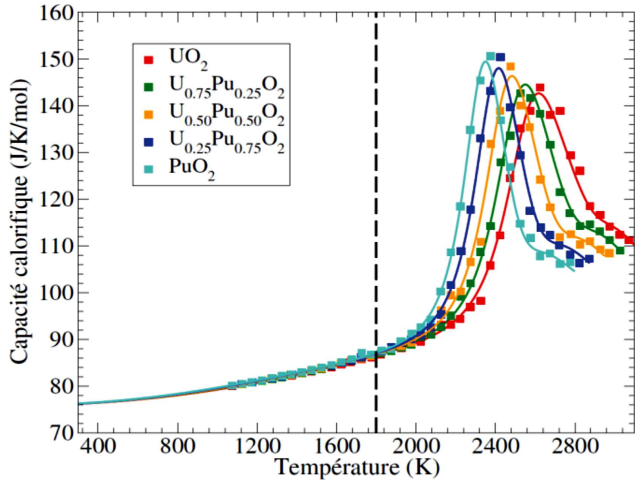

Fig. 5. Heat capacity as a function of temperature and Pu content yielded by atomic-scale calculations and analytical law (solid lines) fitted on these results that were implemented in the GERMINAL fuel performance code.

Laser heating experiments and atomic scale calculations enabled the determination of high temperature and melting properties of (U,Pu)O_2, (Pu,Am)O_2, and O_2. Together with literature data and data from the FP7 ESNII+ project, these results improved the thermodynamic modelling of the (U–Pu–Am–O) system [22]. The specific heat of (U, Pu)O_2 was also evaluated using atomic scale calculations (see Fig. 5), yielding information at very high temperatures and over the full composition range, which is very difficult to measure experimentally [23].

Atomic scale calculations provided further insight into the elementary processes of formation and migration of defects in (U,Pu)O_2 and a new diffusion model for plutonium in MOX fuel and an associated mobility database were developed [24]. In addition, diffusion couples were designed to enable refined experimental measurements of diffusion coefficients.

Diffusion coefficients of inert gases Xe, Kr, and He in fresh UO_2 and MOX were determined using a combination of experimental techniques and modelling methods, from the atomic to the grain scale [25]. Finally, MOX fuel samples from past irradiation campaigns with various Pu contents and at various locations of the pellet, i.e., subjected to different burnups and irradiation temperatures, were characterised using inter alia electron microscopy, down to the nanometer scale.

Complementary techniques and methods were combined to a precise control of materials and test conditions to determine mechanical properties and get further insight into the elementary processes governing their evolution. Elastic properties, ductile-fragile transition and ultimate strength in MOX single crystals as functions of

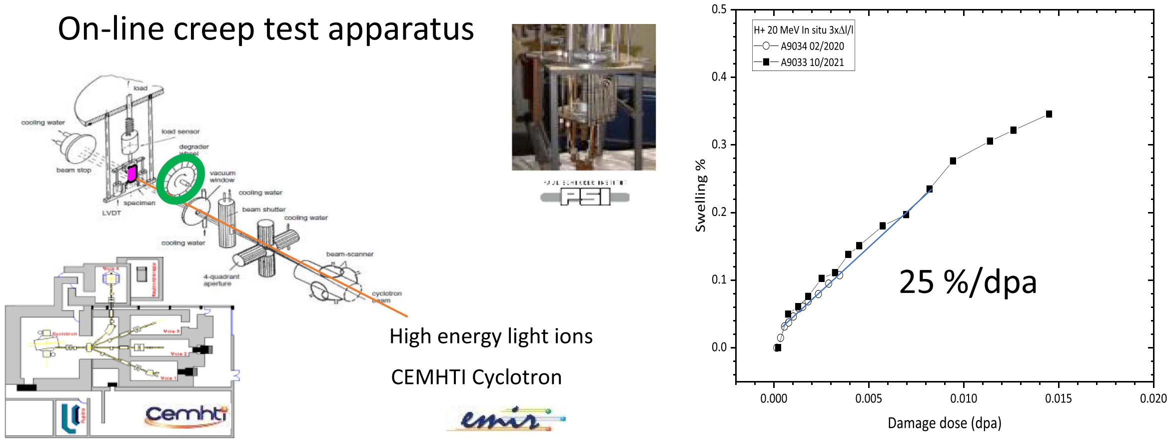

Fig. 6. Apparatus for online creep test under ion irradiation and swelling as a function of damage dose on UO_2 polycrystalline sample.

Pu content, temperature and irradiation dose were studied using atomic scale simulations [26]. Then, thermal creep in UO_2 under controlled conditions (in particular the oxygen partial pressure [27]) was measured in a dedicated setup, while new micro and nano-indenters were used to determine the room temperature elastic properties and micro-hardness at the grain scale of well-characterized fresh MOX fuel samples.

Irradiation-induced swelling in UO_2 was studied in situ using ion irradiation at the CNRS cyclotron in Orléans and MOX in the HFR reactor in Petten. As shown in Figure 6, macroscopic swelling of UO_2 was proved to increase with damage dose, in agreement with the trends shown by simulations and post-irradiation examinations [28]. In addition, deformation was recorded in situ in MOX fuels irradiated under very small temperature gradients in the HFR reactor for 6 months.

INSPYRE also improved significantly the knowledge of the "Joint Oxyde-Gaine" (JOG) layer, which is formed by the migration of volatile fission products, in particular caesium, tellurium, iodine and molybdenum, from the centre to the periphery of the fuel pellet. The incorporation and transport properties of Cs and I in MOX fuel were evaluated using electronic structure calculations. Thermodynamic data on fission product compounds in the chemical system (Cs–I–Te–Mo)–(U–Pu–O) were measured and calculated at the atomic scale [29]. The thermodynamic models on the Te–U, O–Te–U, Mo–O–Te, Cs–Mo–O, Cs–Te–O and Cs–Mo–Te–O sub-systems were then improved using these results.

Finally, properties such as melting temperatures of phases containing U, Pu, Fe and O (PuO_2–Fe_3O_4 system), which form from the interaction between MOX and cladding in the case of a severe accident, were measured for the first time using an advanced laser heating setup. In addition, a novel experimental setup enabled new data to be gathered on the liquid miscibility gap of the Fe–U–O system, in which two immiscible liquid oxide and metallic phases coexist. Thermodynamic models of the U–Fe–O and Pu–Fe–O systems were then derived using these experimental data.

4.2 Advances in the simulation of nuclear fuels

Fuel performance codes used to simulate the behaviour of Gen IV fuels under irradiation were improved using the results presented above. Physics-based correlations giving melting temperature and thermal conductivity versus fuel temperature, Pu and minor actinide content, deviation from stoichiometry, porosity and burn-up were developed for MOX and minor actinide-bearing MOX fuels under GEN IV reactor relevant conditions [30]. Several physics-based models were implemented in the SCIANTIX grain-scale module to improve the description of fission gas and helium behaviour in MOX fuels [31]: (1) a burn-up model to evaluate helium production in MOX; (2) a reduced order model of fission gas diffusion in columnar grains; (3) a model for the intra-granular helium behaviour that accounts for helium diffusivity, solubility and interaction with other fission gases; (4) an improved description of the formation of the High Burn-up Structure and the corresponding porosity evolution at the periphery of fuel pellets. Then, improved correlations were obtained for the MOX thermal expansion and Young's modulus as functions of fuel temperature, Pu content, porosity and deviation from stoichiometry. A 3D micro-mechanical model based on representative volume elements, which includes a description of the fuel rupture behaviour, was also developed for both normal operation and off-normal conditions.

The models and correlations developed in the project were used to improve three major European fuel performance codes: GERMINAL, developed by CEA, MACROS developed by SCKCEN, and TRANSURANUS, developed by JRC with the support of academic organisations. All of them were coupled with the SCIANTIX grain-scale module for inert gas behaviour [32]. The improved versions of these codes were then assessed by simulating the three past fast-neutron irradiation experiments SUPERFACT-1 (see Fig. 7), RAPSODIE-I and NESTOR-3. In addition, data obtained in the second half of the project are available to further improve models and codes.

The code validation against local and integral experimental data reveals harmonized predictions of fuel

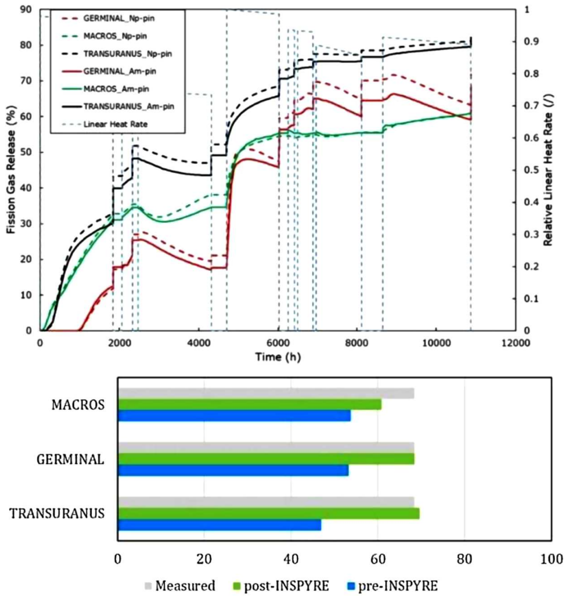

Fig. 7. (a) Relative linear rate and fission gas release at peak power node yielded by improved FPC. (b) Integral fission gas release yielded by pre and post-INSPYRE versions of FPC and comparison with experimental data.

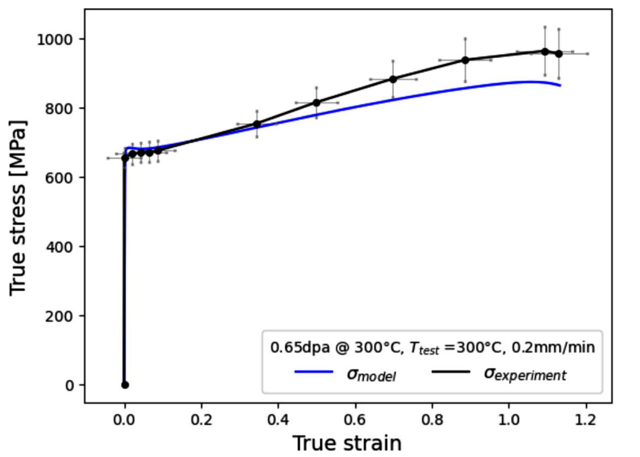

Fig. 8. Simulation of tensile test on irradiated EUROFER97 (0.65 dpa@300 °C): comparison of simulated and experimental true stress vs. true strain curves.

restructuring (as fuel inner void formation). In particular, fuel central temperature predictions are now more consistent between the various codes [33].

4.3 Simulation of ESNII reactor cores

The new versions of the codes were used to simulate normal operation conditions in the ASTRID sodium fast reactor prototype [34], as well as normal and transient conditions in the LBE-cooled reactor of MYRRHA [35]. This enabled the evaluation of the safety margins of the fuel designs (e.g., margin to fuel melting, cladding plasticity) under relevant conditions.

5 M4F: bringing together fusion and fission materials communities to predict the behaviour of ferritic-martensitic steels under irradiation

The M4F project (Multiscale Modelling for Fusion and Fission Materials), which ended in December 2021, was partially funded by the Euratom research and training work programme 2014–2018. It brought together fusion and fission materials research communities to work on the prediction of irradiation-induced microstructural damage and deformation mechanisms of irradiated ferritic/martensitic (F/M) steels, applying a multidisciplinary approach that integrates modelling and experiments at different scales. The main objectives were:

- to develop physical understanding and predictive models of the origin of localised deformation under irradiation in F/M steels and its consequences on the mechanical behaviour of components. This is meant to set the basis for the future elaboration of physically-motivated, non-over-conservative design rules for this class of steels, of use for both fission and fusion applications.
- to identify good practices for the use of ion irradiation as a tool to evaluate radiation effects on materials for modelling and screening purposes, minimising artefacts with respect to neutron irradiation experiments and allowing the evaluation of not only microstructural changes but also mechanical property changes.

The rationale of these objectives, reviewing past work and summarizing research pathways and first results of the M4F project, is the subject of reference [36], while the overall results are summarized in its Final Report [37]. Here we, therefore, provide only a brief highlight of the main results of the project with respect to the above objectives, emphasizing result exploitation and impact aspects.

The project impact concerns two main items:

(1) cross-fertilization between fission and fusion;
(2) overcoming bottlenecks that are limiting developments in fission and fusion.

In connection with cross-fertilization, a continuous effort was made to identify and disseminate cross-cutting research activities of equal interest for fission and fusion applications. Thanks to this effort, the spectrum of these commonalities has progressively widened over time. The pioneering role of the project is proven by the fact that synergies between fission and fusion are currently being sought for also by the IAEA [38]. The outcome of the M4F project in terms of the identification of commonalities between the two materials communities will certainly impact the outcome of this IAEA effort.

Concerning the goal of overcoming the bottlenecks that are limiting developments in fission and fusion, it has

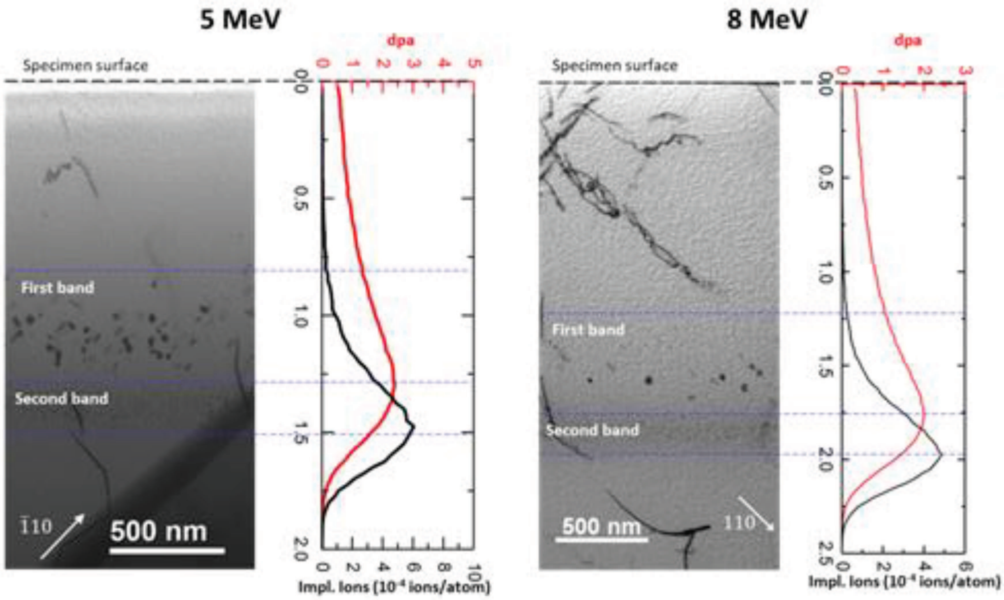

Fig. 9. Ion irradiation damage for two different beam energy values (5 and 8 MeV) as a function of depth: transmission electron microscopy micrographs; dpa and implanted ion profiles calculated.

to be evaluated in terms of advancing towards the two above-stated goals.

Regarding the first one, the problem of plastic flow localization has been addressed covering all scales, from the study of elementary processes concerning dislocation motion in the matrix, through obstacles [39] and across grain boundaries [40,41], using atomistic simulation techniques, to dislocation dynamics [42] and finite element approaches [43–47]. In particular, the visco-plastic modelling approach developed in [45–47] allows the simulation of flow localization in F/M steel structures under neutron irradiation, taking into account finite strains and ductile damage. The model is a powerful tool for the assessment and development of new criteria for immediate plastic flow localization and can also be used to assess other failure modes caused by ductile damage. In case of irradiation causing loss of ductility, it predicts immediate local fracture due to exhaustion of ductility and its dependence on triaxiality. As an example of application, Figure 8 shows how the model can reproduce to a good approximation the experimental true-stress/true-strain curve of irradiated EUROFER97.

Advances were made also in the direction of identifying good practices for ion irradiation experiments [48], with the support of advanced microstructure evolution models [49–51]. The importance of choosing a high ion beam energy value, to mimic as much as possible neutron irradiation, has been clearly evidenced. A characteristic pattern of defect bands linked to the dpa and to the implanted ion profile has been identified, as shown in Figure 9.

One of the bands, between the surface and the damage peak, "safely" resembles the microstructure that is observed under neutron irradiation, provided that the Fe-ion beam energy is $\geq$5 MeV [48]. 8 MeV also give neutron-closer results than 5 MeV in terms of solute-rich cluster formation, but differences are detected as compared to irradiations performed with 5 MeV. It is the first time that the influence of ion energy on the microstructural features has been observed [52]. For the interpretation of the experiments, three microstructure evolution models were developed which, combined, can provide a complete description of the radiation-induced microstructure under neutron and also ion irradiation, including all the specific features of the latter [49–51].

The project included also an important activity on nanoindentation as a tool to evaluate mechanical property changes due to irradiation using ion-implanted specimens [53–56], which are only affected within a depth of a few μm from the surface. In connection with this, the publication of the CEN NATEDA (NAnoindentation TEsting DAta) Workshop Agreement [57] represents an important precedent for the standardization of nanoindentation testing, as a tool for the characterization of the mechanical behaviour of ion-irradiated specimens.

6 Summary and conclusions

GEMMA, INSPYRE and M4F represent examples of multidisciplinary projects with similar goals and approaches, but applied to different materials and conditions, showing the cross-cutting character of these approaches. GEMMA was mainly dedicated to the qualification of structural materials in corrosive environments, stress relief and irradiation effects. INSPYRE and M4F had a heavier modelling component, with a view to improving engineering tools, such as fuel performance codes or component design codes. In the three projects, advanced modelling tools were combined with microstructure examination and experimental measurements in order to improve our level of understanding of the mechanisms and rationalise collected data, enriching experimental data with data obtained from models. These and other cross-cutting materials science approaches, organized into five research lines, constitute the warp, while materials classes constitute the weft, on which the SRIA of ORIENT-NM is being built. In addition, all projects had an intensive and partly common education and training programme not described here, which corresponds to another important cross-cutting activity. It is expected that, by centralising these activities within the same initiative, such as a co-funded partnership, they can maintain their continuity, while benefitting on the one hand from cross-fertilisation and on the other hand from a single management and coordination structure.

Conflict of interests

The authors declare that they have no competing interests to report.

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Author contribution statement

The four authors wrote the manuscript and coordinated the reported projects. The content of the work is the merit of the long list of project participants.

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