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F-BRIDGE

Collaborative Project

Co-funded by the European Commission under the
Euratom Research and Training Programme on Nuclear Energy
within the Seventh Framework Programme

Grant Agreement Number: 211690
Start date: 01/03/2008 Duration: 48 Months
www.f-bridge.eu

Final Project Report

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F-BRIDGE – R-011 – revision 0 – Issued on 20/06/2013 by CEA



F-BRIDGE project – Grant Agreement Number: 211690
 Basic Research in support of Innovative Fuels Design for the GEn IV systems
 EC Scientific Officer: G. Van Goethem

Document title	Final project report
Author(s)	Carole Valot, Marjorie Bertolus (CEA), Rudy Konings, Joe Somers (JRC-ITU), Sander de Groot (NRG) with the contribution of all participants
Number of pages	47
Document type	Final project report
Work Package	WP0-1
Document number	R-011 – revision 0
Issued by	CEA
Date of completion	20/06/2013
Dissemination level	Restricted to the partners of the F-BRIDGE project

Summary

This report is the final report of the F-BRIDGE collaborative project (2008-2012). It summarizes the context and objectives of the project, the activities of the 19 partners, the main scientific and technical results obtained and their potential impact.

Approval

Rev.	Date	Short description	First author	Deputy-coordinator
0	06/2013	First issue	C. Valot, CEA 17/06/2013	M. Bertolus, CEA 20/06/2013

Distribution list

Name	Organisation	Comments
G. Van Goethem	EC DG RTD	
All technical participants	F-BRIDGE	

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1 Final publishable summary report

1.1 Executive summary

The F-BRIDGE project, whose acronym stands for “Basic Research in support of Innovative Fuels Design for the GEn IV systems”, took place over the period 2008-2012. It sought to bridge the gap between basic research and technological applications for nuclear fuel systems. One of the challenges for the next generation of reactors is to significantly increase the efficiency in designing innovative fuels. The main objective of the F-BRIDGE project was therefore to complement the classical empirical approach by a more physically-based description of fuel and cladding materials which is essential to reach a better knowledge and by doing so to enable a better prediction, leading itself to a rationalization of the design process and a better selection of promising fuel systems. F-BRIDGE relied on the complementary expertise of 19 partners: nuclear and non-nuclear research organisations, universities, a nuclear engineering company, as well as technology and project management consultancy small and medium enterprises. F-BRIDGE produced extensive and consistent scientific and technical results.

One of the main objectives of F-BRIDGE was to perform basic research investigations on nuclear ceramic fuels and their cladding. It took advantage of the use of innovative experimental and modelling techniques in a consistent multiscale approach from the atomic to the macroscopic scale and made significant breakthroughs in the detailed knowledge of ceramic fuels and cladding behaviour for the performance and safety optimization. The project contributed to produce key basic data and identify relevant mechanisms that are to be used for a better prediction of fuel behaviour. Knowledge on the atomic transport properties of oxygen, fission products and helium in fuels, as well as of silver in SiC cladding, was considerably improved, and data were either updated or acquired through experimental characterisation studies. Micro-structural changes induced by gas bubble formation and growth, as well as damage produced by irradiation and their effect on transport properties were also investigated in depth. Regarding the atomic scale modelling of transport properties and micro-structural changes in carbides and nitrides, F-BRIDGE studies improved the description of the elementary mechanisms involved in the behaviour of these materials under irradiation and contributed to generate basic data. Finally, innovative experiments and advanced modelling using the CALPHAD method largely contributed to improve the knowledge on the thermodynamical stability of various fuel systems and their chemical interaction with their environment.

A significant contribution of F-BRIDGE was the integration effort between the various actors involved which improved the links between basic research and applied issues, scientist and end-users, investigations at various scales from atomic to macroscopic, modelling and experiments, experts and students. Data request lists gathering key technological issues, pending scientific questions and corresponding basic research investigations were built from the fruitful interaction between F-BRIDGE participants and industry representative members of the user group, showing the contribution basic research can make to solve key technological issues. Significant progress was made in the validation of atomic scale modelling methods and approximations used on fuel materials, which has contributed to improve their reliability. In addition, a special effort has been put to improve the link between scales. The mesoscopic scale was identified as a key scale since it bridges data and mechanisms obtained at lower scales to the fuel performance codes at macroscopic scale. The multiscale modelling exercise on transport properties in uranium dioxide, which demonstrated that electronic structure and empirical potential calculations can be used to obtain precise data to feed higher scale models and help interpret experiments on fuels, is one of the major successes of F-BRIDGE. The project also highlighted the importance of coupling experiments and modelling in an efficient way. Complementary to integral irradiations, separate effect studies performed in well controlled and various irradiation conditions, out of as well as in-pile, were identified as key experiments to contribute to a better understanding of phenomena occurring under irradiation and to produce data for the modelling validation. F-BRIDGE demonstrated a first success in updating existing fuel performance codes by introducing into them advanced material properties and models obtained from basic research and the multiscale modelling approach.

Applied research was moreover performed to assess and improve 'sphere-pac' fuel, a composite-ceramics concept which had shown promise. F-BRIDGE project has shown the interplay between modelling and technology, drawing on fundamental physics and chemical approaches and coupling them to detailed economic impact analysis to demonstrate the feasibility of an advanced fuel concept such a sphere-pac. Quality assurance has also been shown as a key component ensuring the reliability of reactor fuels. The F-BRIDGE project connected advanced experimental characterization methods operating at various size ranges (nm to mm), proving beyond doubt that a basic scientific approach is a key element to underpin quality of nuclear fuels. F- BRIDGE finally enabled the establishment of a joining technology for an advanced cladding material, with potential gains in the quest for a robust accident tolerant nuclear fuel, by establishing fundamental thermochemical properties of a soldering material to join SiC components.

F-BRIDGE has had a high level of knowledge dissemination and valorisation as demonstrated by the numerous peer-reviewed articles – approximately 80- and the comprehensive deliverables published during the project. F-BRIDGE was also very active in the international community by participating in the most important international conferences in the field (NuMat, MRS, MMSNF...) as well as in important instances as the OECD/NEA working party on multiscale modelling of nuclear fuels and materials. It had also close relationships with other European projects (CP-ESFR, PERFORM 60, GETMAT, ACTINET I3,...). A proof of the high quality of the work performed in F-BRIDGE and attractiveness to young scientists is the large number of PhD students and post doctorate associates - 34 - involved in the project. Regarding education and training activities, two successful schools were organized during the project and contributed to strengthen the links between senior scientists and students: the first one was dedicated to “Ceramic nuclear fuel and cladding materials” and the second one to “the synergy between modelling and experiments for the investigation of nuclear fuels and materials under irradiation”. Finally, a particular success of F-BRIDGE is the fruitful interaction with the international scientific advisory committee members which highlighted the quality of the work performed in the project and made constructive recommendations.

All the F-BRIDGE partners contributed effectively to lay the stones joining both end of a bridge between basic research and applied issues, improving knowledge and enabling a better prediction of fuel behaviour and selection of promising fuel systems. Even if a challenge for the future is the frequent use of such a bridge, its construction represents the exceptional success of the F-BRIDGE European project.

1.2 Project context and objectives

International effort is on-going to increase the efficiency in designing innovative fuels both to improve performance and safety of current fuel systems and to design those for tomorrow. At the time of F-BRIDGE proposal, European experts had an adequate knowledge of conventional fuel manufacturing and its behaviour under operating conditions encountered during 50 years of industrial application and R&D activities. For innovative fuel systems, however, the empirical approach had reached its limit and could not be easily extrapolated to new materials, new environments or new operating conditions because the basic underlying mechanisms governing manufacturing, behaviour and performance remained poorly understood. One of the challenges at the time was to complement the empirical approach mainly used for fuel development and qualification by a physically based description of ceramic fuel and cladding materials. To do so, the F-BRIDGE project aimed at bridging the gap between basic research and technological applications for generation IV nuclear reactor systems. Advanced modelling and separate effects experiments were planned and expected to provide more exact physical descriptions of ceramic fuels and cladding at all relevant scales from the atomic to the macroscopic scale. Besides a general approach on ceramic materials, F-BRIDGE also focused on assessing and improving sphere-pac fuel, a composite-ceramics concept which had shown promise.

To achieve its objective, the project was broken down into four main areas:

- **Domain 1: Basic research: experimental simulation and modelling of fuels and SiC cladding from the atomic to the mesoscopic scale.** Basic research investigations focused on the generation of missing basic data, the identification of relevant mechanisms and the development of appropriate models. In particular, a multiscale approach in both experimentation and modelling was to be developed to bring further insight into the physical, chemical and mechanical behaviour of fuel materials under extreme conditions of temperature and irradiation.
- **Domain 2: Integration of all scales, transfer between technological issues and basic research.** To be really effective and tackle the most important issues relative to the various Generation IV systems, basic research investigations were to be strongly connected to their clients, i.e. fuel designers and manufacturers. The transfer between technological issues and basic research was aimed at bringing together within the same project materials scientists, engineers and end-users that have a detailed knowledge of critical issues.
- **Domain 3: application to advanced sphere-pac fuel design**
As part of this integration effort, F-BRIDGE aimed at providing an assessment of the benefits and drawbacks of the sphere-pac fuel application to various Generation IV systems.
- An additional important objective of F-BRIDGE was to organise education and training activities. This included meetings and workshops for scientists, design engineers and end-users involved in the project or not, which were to ensure exchange of results and ideas among the participants. Two summer schools for young scientists were also planned to promote research in the field of fuel materials and help to prepare to meet future challenges. Knowledge sharing between F-BRIDGE experts and young scientists via the training of PhD students and post-doctoral associates involved in the project was meant to be actively encouraged as well.

1.2.1 *Domain 1*

The goal of the domain 1 of F-BRIDGE was to undertake a set of basic research actions on fuel and ceramic cladding materials in a consistent approach coupling experimental simulation and modelling at the relevant scales. This approach appeared to be the only way to de-correlate the complex phenomena occurring in the

fuel and ceramic cladding under irradiation and to get further insight into basic phenomena and mechanisms. The data obtained could then be used as direct input or for validation purposes in predictive numerical simulation of the macroscopic fuel behaviour under irradiation. Experimental simulation and modelling were intended to be developed in close relationship in order to maximise the impact of their results.

The experimental simulation based on “separate effect studies”, involving both active and model materials, was meant to be complemented by results from in-reactor irradiation testing (not included in the project) and dedicated post-irradiation examinations (PIE). Adequate characterisation techniques probing structural stability, atomic transport properties and thermo-mechanical properties were planned to be used to assess the mechanisms involved in fuel behaviour under normal and off-normal conditions. A set of dedicated experimental tools was chosen to study the effects of temperature and radiation, as well as the potential chemical interactions inside the fuel and between fuel, cladding, coolant and thermal bond materials.

The modelling investigations focused on the atomic scale of actinide nitride and carbides, as well as of silicon carbide, and involve electronic structure calculations or the use of empirical interatomic potentials.

The use of these methods had just begun in the field of nuclear fuel because of difficulties due to the specific properties of fuel materials. Nuclear fuels and ceramic cladding are usually insulators or semi-conductors and have therefore specific thermo-mechanical and transport properties. The defects generated by irradiation are also significantly more complex than in metals, for instance because of their electric charge. Finally, the modelling of nuclear fuels is particularly challenging because of the complex behaviour of 5f electrons in actinide compounds. But since modelling tools and computing capacities are improving continuously, they were expected to bring a decisive contribution to the knowledge of nuclear fuel behaviour under irradiation.

Finally, thermodynamics modelling was identified as a powerful and essential technique to assess the stability of compounds through phase diagram calculations and get further insight into the interaction mechanisms between the fuel and fission product compounds, as well as between the fuel and its direct environment (cladding).

1.2.2 Domain 2

The objectives of F-BRIDGE Domain 2 as formulated in the project “description of work” were to ensure the transfer and integration between technological issues of Generation IV systems and basic research:

- Ensure the bi-directional transfer and translation between technological issues of Generation IV systems and basic research by bringing together people from fuel material science and clients who know the critical issues relating to fuel manufacturing and fuel behaviour under irradiation,
- Ensure the integration of scales by evaluating the impact and feedback of basic research results on innovative fuel design, manufacturing, in-pile behaviour prediction and on the design optimization of irradiation experiments.

Within domain 2, these objectives referred to integration between various scales and between various technical and disciplinary levels. They were intended to be achieved step-wise in four areas:

- integrate technical requirements from nuclear fuel industry with scientific and technical R&D efforts in F-BRIDGE
- integrate the various modelling scales, from the atomic scale to the microscopic and mesoscopic scales. In particular, a multiscale modelling exercise on the atomic transport properties in uranium dioxide, which mobilised a wide range of techniques from the atomistic scale with electronic structure calculations or the use of empirical interatomic potentials to the meso- and macroscopic scales, was planned.
- integrate modelling and experimental efforts
- integrate mesoscopic modelling in fuel performance codes, and integrate sphere-pac fuel performance codes with fuel performance codes in which sphere-pac had until then been excluded

1.2.3 Domain 3

The domain 3 of the F-BRIDGE project focused on the investigation of the sphere-pac concept and on its application as innovative fuel for GEN IV systems. It started from the intensive investigations performed on sphere-pac for LWR fuel in the 70's and 80's, as well as from newer promising results on the addition of molybdenum spheres to sphere-pac fuel, cermet sphere-pac concepts and liquid metal bonding, and expanded possibilities for improved (thermal) performance. In particular, innovative procedures of fuel microsphere fabrication by sol-gel technique were planned to be established, promising high conductivity thermal bond materials be tested, and the benefit of (liquid) metal bonded sphere-pac fuel be evaluated. The additional and stringent requirements set by the Generation IV framework, induced by increased safety and sustainability demands, seemed to make the advantages of sphere-pac fuel application even more significant.

The sphere-pac fuel types proposed to be evaluated were intended to be beyond the state of the art in meeting the objectives and requirements of Generation IV systems. The large amount of sol-gel and sphere-pac fabrication knowledge and the large modelling experience of several partners of the F-BRIDGE project were to be called upon to enable a precise evaluation of the potential and disadvantages of the fuel types considered from a core physics, thermomechanical and chemical point of view, making use of the integration and basic research activities as much as possible. A number of basic research items contributing to increased effectiveness of sphere-pac fuel design were already identified, but it was expected that more multiscale chains could be found that would contribute to the optimal approach of fuel design and the optimal sphere-pac fuel types for Generation IV systems. Both the new approach and the sphere-pac fuel types that would be obtained were expected to be beyond the state of the art.

1.3 Main S&T results

F-BRIDGE produced extensive and consistent scientific and technical results, as demonstrated by the numerous peer-reviewed articles - approximately 80 - and the comprehensive deliverables published during the whole project duration. The high quality of the scientific work performed in F-BRIDGE was also demonstrated by the large number (34) of PhD students and post doctorate associates involved in the project. In addition, F-BRIDGE results were made particularly visible through the numerous scientific presentations at relevant international conferences, as well as during F-BRIDGE final international workshop.

The main scientific and technical results are presented below for the three technical domains.

1.3.1 Domain 1

To reach the objectives of the domain described in section 1.2.1, advanced modelling and characterization tools were developed at various scales. Such investigations successfully enabled us to:

- generate important missing basic data or confirm existing ones such as diffusion coefficients, melting temperatures or thermodynamic data. F-BRIDGE achieved this objective by performing new measurements in well controlled conditions (oxygen potential for fuels for instance) and samples (chemical composition, impurity rates, density,...) to improve the reliability and confidence in the obtained data. F-BRIDGE used dedicated and innovative characterization techniques that are at the cutting edge for ceramic fuel and cladding (among them electrical conductivity, laser heating, Knudsen cell mass spectrometry, TEM, positron annihilation spectroscopy, high temperature X-ray diffraction, NMR, tomography, techniques using synchrotron radiation or ion beams,...). The characterization went toward a finer and finer description of the phenomena involved down to the atomic scale. This objective was also achieved through application of atomic scale methods, especially on uranium carbides and nitrides on which experiments are difficult or even impossible.
- de-correlate and identify the relevant mechanisms involved under irradiation through a coupled modelling and experimental approach. Even if fuel materials are challenging to characterize and model, F-BRIDGE obtained impressive results that could not have been obtained without such a coupled approach. These results have demonstrated the complementarity of the two types of studies and the synergy that can be achieved when they are used jointly, experiment contributing to modelling validation and modelling contributing to the interpretation of experimental data.
- develop the appropriate models at various scale and improve them with a more and more science-based approach supporting the macroscopic simulation of fuel behaviour under irradiation to reach a better prediction. Methods at the cutting edge in the field such as electronic structure calculations, empirical potential methods, rate theory, CALPHAD, were used.

Domain 1 was broken down in five technical work packages: the first two WP (1-1 and 1-2) were dedicated to the study of transport properties and microstructural changes under irradiation of fuels and SiC cladding, the first one focusing on the experimental characterization, while the second was dedicated to modelling. The latter work package focused on carbide and nitride fuel and cladding and had a lot of interactions with its counterpart WP of Domain 2 dedicated to the multiscale modelling of UO₂. The other three work packages were dedicated to the investigation of thermodynamic stability and chemical interactions, using both experiments and modelling. WP1-3 aimed to improve the thermodynamics description of the U-Pu-O-C systems, WP1-4 studied the impact of minor actinides and fission product on phase diagrams, and WP1-5 was dedicated to the fuel-environment chemical interaction. The results obtained in the various WP are detailed below.

1.3.1.1 WP1-1: Experimental characterisation of transport properties and micro-structural changes in fuels and SiC cladding

Knowledge on the atomic transport properties of oxygen, fission products and Helium in fuels, as well as of silver in SiC cladding, was considerably improved and data were either updated or acquired through the experimental characterisation studies performed in F-BRIDGE. Micro-structural changes induced by gas bubble formation and growth, damage produced by irradiation and their effect on transport properties were also investigated in depth.

- **Irradiation induced diffusion of He and I in UO₂ was studied using a large panel of techniques under controlled experimental conditions** (preparation, irradiation conditions, annealing) and contributed to build a much clearer picture of helium behaviour in UO₂. The results highlighted the role of radiation damage and temperature in damage recovery processes (D111). TEM experiments were also performed to find the conditions of helium bubble formation in UO₂. The evolution of helium position in UO₂ lattice and the recovery of the oxygen sublattice during annealing were investigated using canalised Rutherford Backscattering and nuclear reaction analysis measurements. To understand the role of vacancy type defects in the migration mechanism of helium, positron annihilation spectroscopy was used to follow the evolution of vacancy complexes with temperature. Finally, complementary isothermal and isochronal helium release experiments were performed in infused UO₂ single crystals to understand the role of stoichiometry on helium solubility (D115).
- **The thermal diffusion of oxygen in UO₂ was assessed from self-diffusion coefficient and electrical conductivity measurements.** The dependences of the experimental data upon oxygen potential and sample impurity content demonstrate, by comparison with basic point defect and diffusion theory, that oxygen migration occurs via an interstitial mechanism under the extrinsic conditions examined. The experimental activation energy obtained for oxygen self-diffusion in uranium dioxide compare very favourably with electronic structure calculations performed in Domain 2. This investigation is a good example of studies linking first principles theoretical approaches and experimental measurements (D112).
- **The effect of α -damage on the thermophysical properties of UO₂ was investigated using samples doped with ²³⁸Pu.** The measurements showed that the degradation of the diffusivity with increasing α -dose is not linear, and saturation occurs at relatively low doses. A correlation quantifying this degradation was proposed (D113).
- **The radiation enhanced diffusion of chlorine-37 in UO₂ was studied** (D114).
- **First uranium carbide samples were manufactured and characterized.** UC pellets were fabricated using a carboreduction process under controlled atmosphere. Nuclear reaction analyses were applied for the first time to scan the oxygen concentrations at the surface. Raman characterizations were used to probe the presence of impurity phases. Preliminary measurements were performed with positron annihilation spectroscopy in order to evaluate the feasibility of using this technique to study the properties of vacancy defects in UC as it was done in UO₂ (D116).
- **The microstructure of irradiated SiC was characterized.** Point defects and amorphisation of crystalline SiC, interfaces in SiC/SiC composites, as well as the influence of the dimensionality were investigated using nuclear magnetic resonance, Raman spectroscopy and X-ray absorption spectroscopy (D117).
- **Ag diffusion in SiC** was investigated thanks to Raman spectroscopy, X-ray microtomography and scanning and transmission electron microscopy. It was clearly demonstrated for the first time that silver diffuses by grain boundary diffusion and that neither excess silicon nor grain size are relevant to the diffusion of silver as was previously speculated (D118).

1.3.1.2 WP1-2: Atomic-scale modelling of transport properties and micro-structural changes in carbides and nitrides

Regarding the atomic scale modelling of transport properties and micro-structural changes in carbides and nitrides, F-BRIDGE studies improved the description of the elementary mechanisms involved in the behaviour of these materials under irradiation and contributed to generate basic data.

- **First-principles electronic structure investigations were performed on:**
 - **Bulk nitride:** The behaviour of point defects and of oxygen impurities in UN were studied using electronic structure calculations. The incorporation of various fission product elements in UN was also investigated and complemented with results obtained for a (U,Zr)N solid solution. The analysis of vacancy mobility was used for an assessment of the effect of oxygen impurities on thermal creep in the TRANSURANUS fuel performance code (D121).
 - **Bulk actinide carbides:** Elementary mechanisms governing the evolution of the fuel material under irradiation at the atomic scale were determined and allowed us to get further insight on the behaviour of defects, fission products and oxygen, as well as the effect of non-stoichiometry on this behaviour (D122).
 - **Uranium nitride surface:** Formation energies, geometries, charge density distribution, migration and interaction energies were calculated. The incorporation of oxygen into surface N vacancies, which is the first step in oxynitride formation, was also investigated (D123).
- **The effects of irradiation and diffusion near SiC grain boundaries were investigated using empirical potentials.** Classical molecular dynamics simulations of displacement cascades were performed on nano-crystalline SiC and the diverse trends associated with initial velocity directions and grain orientations were compared to bulk results (D124).

1.3.1.3 WP1-3, WP1-4, WP1-5: Thermodynamics of U-Pu-O-C fuel systems, impact of minor actinides and fission products on phase diagrams and fuel-environment chemical interaction

Innovative experiments and advanced modelling using the CALPHAD method done in F-BRIDGE largely contributed to improve the knowledge on thermodynamics stability of various systems of fuels and their chemical interaction with their environment

- **Rigid lattice thermodynamical calculations were performed.** Density Functional Theory calculations on uranium and plutonium carbides were done preliminary to the development of pair interatomic potentials for the U-Pu-C system. The structural and elastic properties of uranium and plutonium mono-, di- and sesquicarbides were calculated. The second stage of the study involved the fitting of the DFT results to obtain interatomic interactions on a rigid lattice in the difficult cases of uranium plutonium carbides and oxides. A set of effective cluster interactions is now available to perform rigid lattice thermodynamical calculations in the future (D131 rev 0 and 1).
- **An updated phase diagram of the U-C system was developed:** Both solidus and liquidus phase relations within the U-C binary system were established by combining, experimental work carried out in a wide range of temperatures and compositions and thermodynamic calculations using the Calphad method. The description emphasises two different behaviours of the U-C binary system, one corresponding to a metastable phase-diagram and one to the stable phase-diagram (D133).

- **The high temperature behaviour of the U-Pu-O system was investigated** with particular focus on the vaporization and melting behaviours. (U, Pu) MOX pellets were prepared by blending pure dioxide powders, pressing and sintering. Laser heating under controlled atmosphere was used for the melting behaviour investigation. Preliminary studies on their vaporization were performed by Knudsen cell effusion mass spectroscopy. The results suggested that whereas the melting points of pure PuO₂ and of Pu-rich (U, Pu) MOX are considerably higher than previously assessed, the formation of a stable gas phase cannot be neglected for these compounds, even at temperatures below melting (D132).
- **The U-Pu-O-C system was investigated experimentally and using the Calphad modelling method.** A thermodynamic model was derived for the (U,Pu)O₂ oxide and the (U,Pu)C carbide fuels to describe consistently both phase diagrams and thermodynamic data of the phases involved in the U-Pu-O-C system. The experimental liquidus data measured at JRC-ITU by laser heating were taken into account. All the available thermodynamic and phase diagram data of the binary and ternary sub-systems are very well reproduced by the model (D134, D135). Besides reproducing existing literature data fairly well and producing original new data, this work stressed the paramount importance of a systematic determination of the effect of oxygen impurities on carbide systems, a type of investigation which has never been carried out on actinide carbides (D136).
- **Selected grey phase compounds were prepared and characterized.** Since the preparation of the mixed phases directly from the pure compounds was unsuccessful, an alternative synthesis route was tested, in which the dioxides were first mixed at 1650°C and then reacted with the BaO at 1200°C. Successful formation of the Ba(Pu,Zr)O₃ mixed perovskite was confirmed by X-ray diffraction (D141). The melting behaviour of selected grey phase compounds was studied using laser heating. Pellets of the pure compounds BaUO₃ and BaPuO₃ were analysed. The melting behaviour of BaUO₃ was found to be more complex than the one of BaPuO₃, probably due to the presence of excess BaO and segregation effects. Novel data were produced for the liquidus and eutectic temperatures of BaPuO₃ (D144).
- **Molecular actinide compounds were studied using *ab initio* methods.** The properties of neutral and cationic neptunium and plutonium oxide molecules, as well as of neutral molecular monocarbides, dicarbides and tetracarbides of uranium, plutonium and americium were calculated. Comparison with available experimental data showed a good agreement for the ionization energies. Due to the limitations of the quantum chemical approach the computed dissociation energies give only qualitative information but enabled us to determine trends within the various series of compounds. The computed geometries, vibrational frequencies and electronic excitation energies will be used to derive the thermal contributions to the thermodynamic properties (D142).
- **The U-Pu-Am-O system was characterized experimentally.** The chemistry of uranium, plutonium and americium in MOX fuel and in particular their oxidation states, was followed and characterized using X-ray diffraction and absorption spectroscopy of (U, Pu, Am)O_{2-x} samples sintered under various oxygen potentials (D143).
- **A thermodynamic database was developed for the U-Pu-Am-Np-O system using the Calphad method** to predict the phase relationships and thermodynamics of mixed oxide fuels containing minor actinides. All the binary sub-systems were described on the basis of the available experimental data. For the ternary sub-systems, ternary interaction parameters were adjusted to improve the description of the available experimental data for the U-Pu-O, Am-Pu-O and Am-Np-O systems. The vapour pressures measured recently for the Am-O and Pu-Am-O systems were taken into account (D145).
- **The U-Mo-C phase diagram was investigated experimentally.** Isothermal sections were established in a wide range of temperatures and compositions. The precise measurement of the Solidus points allows for a rigorous assessment of the thermodynamic parameters, as well as of the invariant reactions encountered in the ternary system (D146).

- **The U-Pu-Si-C phase diagram was investigated experimentally and using modelling.** The (U-Si-C) ternary phase diagram at 1000°C and experimental points in the quaternary (U-Pu-Si-C) system were determined experimentally and were shown to exhibit new features. A thermodynamic database on the U-Pu-Si-C system was developed using the Calphad method to predict the phase relationships and thermodynamics of mixed carbide fuels and the chemical interaction with a clad made of SiC/SiC_f composite. The ternary sub-systems were calculated by extrapolation from the binaries (D151, D152).

1.3.2 Domain 2

The objectives of F-BRIDGE Domain 2 described in section 1.2.2 were achieved step-wise in four work packages:

- WP2-1 integrated the technical requirements from nuclear fuel industry with scientific and technical R&D efforts in F-BRIDGE.
- WP2-2 focused on the different modelling scales, from the atomic to the mesoscopic scale.
- WP2-3 integrated the modelling and experimental efforts, in particular irradiation experiments and post-irradiation experiments.
- WP2-4 put in relation mesoscopic modelling with fuel performance codes, as well as sphere-pac fuel performance codes with fuel performance codes in which sphere-pac had not been included.

The achievements in the various work packages were as follows.

1.3.2.1 WP2-1: Translation of technical issues into basic research investigations

Data request lists gathering key technological issues, pending scientific questions and corresponding basic research investigations were built from the fruitful interaction between F-BRIDGE participants and industry representative members of the user group. It showed the contribution that basic research can make to solve key technological issues.

Data request lists linking industrial and scientific issues were built from meetings between members of F-BRIDGE and the user group formed by representatives of industrials and utilities.

The extensive amount of information retrieved from the end users was translated into common subjects of generic interest to them, such as stoichiometry, fission product diffusion behaviour, bubble formation and evolution, etc. Subsequently, research activities that could contribute to provide more insight in the various mechanisms that play a significant role in the behaviour and performance of nuclear fuel were identified. The data request lists are presented in the form of a three column table. The first column gathers examples of key technological issues. These key industrial issues are translated into pending scientific questions in the second column. The third column gives a non-exhaustive list of basic research investigations, either performed in the framework of F-BRIDGE or to be carried out in the future, which would provide answers. The data request lists are separated in two parts: the first one addressing light water reactors and the second one concerning Generation IV reactors (D212).

The progress made in the F-BRIDGE, as well as the way multiscale efforts can be of assistance to get further insight into the fuel behaviour in various conditions, and subsequently contribute to safe and efficient operation of existing and new nuclear power plants, was presented to the user group during the F-BRIDGE final international workshop. The user group members expressed their interest in the results obtained in F-BRIDGE and in participating in a potential follow-up of the project, either as user group members or as full partners.

1.3.2.2 WP2-2: Multiscale modelling exercise on uranium dioxide: transport and thermo-mechanical properties

Significant effort was made in F-BRIDGE to evaluate approximations and results of atomic scale methods on fuel materials, as well as to improve the link between scales. The mesoscopic scale was identified as a key scale because it bridges atomistic and macroscopic modelling. The multiscale modelling exercise on transport properties in uranium dioxide is one of the major successes of F-BRIDGE demonstrating that electronic structure and empirical potential calculations can be used to obtain precise data to feed higher scale models and help interpret experiments on fuels.

Extensive work was done in the WP2-2 on the modelling of uranium dioxide from the atomic to the mesoscopic scale, a large part of it being completely new in the field of multiscale modelling. The results obtained were presented in the 6 comprehensive deliverables of the work package.

- **A collective effort of validation of the atomic scale models for the description of UO₂ under irradiation was done** in the first two years of the project, and methodological developments made. Density functional theory, empirical potentials, methods of exploration of potential energy surfaces and simulation of radiation damage using displacement cascades were particularly considered (D221).
- **The transport properties and radiation damage in bulk UO₂ containing defects and/or fission products were investigated.** The creation, migration, recombination and clustering of point defects were determined both in stoichiometric and in non-stoichiometric UO₂. The effect of these point defects on several macroscopic fuel properties, such as lattice parameter or diffusion of oxygen and fission gases, was then investigated. The location, diffusion and resolution of fission gases and helium was also studied to determine the migration mechanisms which lead to the formation of bubbles and are of primary importance to better understand the fuel performance (D222).
- **The transport properties in polycrystalline UO₂ and in the presence of extended defects were studied using empirical potentials.** The objective was to get further insight into the high burn-up structure by investigating the effects of grain boundaries and dislocations on the transport properties of oxygen and uranium, as well as of helium and xenon. The results obtained showed that extended defects have a significant impact on the segregation and diffusion of both intrinsic and extrinsic species in UO₂. Grain boundaries were also shown to have a substantial influence on the evolution during irradiation (D223).
- **The mechanical properties of complex microstructures were also investigated using empirical potentials.** They showed that UO₂ undergoes phase transitions under compressive or tensile load. The analyses of the cracking propagation mode of UO₂ showed a phase transformation at the crack tip, secondary cracks being then initiated in this new phase and coalescing with the main crack. Irradiation damage increases the yield stress and delays the strain at which the UO₂ matrix cracks. A first classical molecular dynamics study of dislocations in UO₂ was also performed (D224).
- **Two mesoscale methods, cluster dynamics and kinetic Monte Carlo, were applied to the diffusion processes in UO₂.** It was shown that these methods enable one to address specific problems that cannot be dealt with by standard mesoscopic models included in fuel performance codes, especially the impact of point defects on the microstructure evolution and gas behaviour. Both studies largely rely on basic data calculated using electronic structure and empirical potential methods or determined through experiments (D225).
- **The multiscale modelling exercise on transport properties in uranium dioxide, a major success of F-BRIDGE, showed the links built between the atomic and mesoscopic scale** by presenting the data calculated at the atomic scale which can be used as input in mesoscale modelling. Atomic scale

modelling methods bring valuable insight, in particular the formation, binding and migration energies of point and extended defects, fission product localization, incorporation energies and migration pathways, elementary mechanisms of irradiation induced processes. The significant results obtained shown that it is now feasible to use electronic structure and empirical potential calculations to obtain precise data to feed higher scale models and help interpret experiments on fuels (D226) .

If a lot of the investigations performed in work package 2-2 concerned the atomic scale, significant progress was made in the calculation of results at larger scales that allow microscopic experimental validation. The work on mesoscale methods has progressed with input from lower scales and made the multiscale approach on UO_2 a reality, as demonstrated in the final deliverable of the WP on the multiscale exercise on UO_2 . Moreover, the links with experimentalists of the project have been strengthened, as is demonstrated by several common articles including modelling and experimental results and the technical meeting between the WP1-1 focused on the experimental investigations and WP2-2 organized in 2011. The results obtained in this work package were reported in 26 articles published in peer-reviewed scientific journals.

1.3.2.3 WP2-3: Best practice guidelines for irradiation test campaigns contributing to multiscale modelling

F-BRIDGE has demonstrated the importance of coupling experiments and modelling in an efficient way. Complementary to integral irradiations, separate effect studies, out of as well as in-pile, performed in well controlled and various irradiation conditions (flux, temperature,...) are key experiments to contribute to a better understanding of phenomena occurring under irradiation as well as produce data for the model validation.

The objectives of this work package were to:

- develop guidelines for dedicated future irradiation tests and post-irradiation experiments (PIE) that would maximise effectiveness in providing the input and validation data suitable and valuable for modelling efforts at the various scales,
- deliver experimental results which would be used as input for modelling efforts, as additional clarification on aspects relevant for modelling, as well as for modelling validation purposes.
- **To achieve these objectives, a first step was to synthesise the lessons learned from the past experiments on advanced fuels (D231).** This review particularly assessed the knowledge related to fuel operation safety derived from past irradiation experiments on nuclear fuel samples and presented the knowledge deficiencies related to safe operation of fast reactor oxide fuel (with minor actinides), carbide/nitride fuel and HTR coated particle fuel. A number of recommendations for future studies on all these fuel types were also made.
- A second step was to review the key material basic data and properties needed for the input and validation of the modelling methods that can be applied to the description of nuclear fuel from the atomic to the macroscopic scale (D232). Complementary modelling methods were considered in this review - electronic structure methods calculations, empirical potentials and classical molecular dynamics, kinetic Monte Carlo, rate theory methods, phase field, dislocation dynamics, finite element analysis, fuel performance codes. The document present on the one hand the input parameters that the various methods or models require and how these parameters can be obtained, and on the other hand the results yielded and how these results can be validated experimentally.
- As an illustration of experimental answer to the modelling validation needs, **the feasibility of using electron back scattered diffraction on irradiated UO_2 to access key information for modelling was**

evaluated (D233). This characterization technique makes the grain and their orientation in the material visible, which enables one to get further insight into the evolution of the material under irradiation at various temperatures. This provides valuable data for modelling and can serve for the validation of modelling approaches.

- Finally, **dedicated irradiation tests and PIE that could effectively contribute to multiscale modelling efforts were presented** (D234). Examples of separate effect experiments and integral fuel testing where the experimental results were confronted with predictions based on modelling were given. Practical guidelines for further dedicated future irradiation tests and post-irradiation characterization that would provide input and validation data at various levels of the multiscale modelling were formulated. Experimental methods and in-core instrumentation currently used in the irradiation experiments were also reviewed.

1.3.2.4 WP2-4: Transfer of basic research and mesoscopic results to macroscopic models and fuel performance codes

F-BRIDGE demonstrated a first success in updating existing fuel performance codes by introducing into them advanced material properties and models obtained from basic research and the multiscale modelling approach.

F-BRIDGE aimed at updating the fuel performance codes for advanced fuels with new material properties and models. To this end, the material properties and models for materials behaviour resulting from the basic research activities planned in work packages 1-1 to 1-3, as well as from the integration work in WP2-2 and WP2-3 were considered for introduction in new versions of fuel performance codes TRANSURANUS and GERMINAL for cylindrical fuel rods and the SPHERE and SPACON codes for spherical particle fuel.

- A first task was to **write a state-of-the-art report about material properties of advanced carbide and nitride fuels** (D241).
- A second objective was the **implementation of updated material properties in fuel performance codes**. Recently obtained material properties for oxide, nitride and carbide fuels required for the safety assessment and detailed fuel design for pellet-type and spherical particle fuels were implemented in the TRANSURANUS code. The new version of the code was successfully compared against experimental results from the SUPERFACT experiment in the Phenix FBR (D242, D243).
- The third objective was **the implementation of new models in the TRANSURANUS code**. Among the fuel property models available in the SPHERE-3 code, a list of UO₂ models needed to be implemented in TRANSURANUS was proposed: two models for Poisson's ratio and emissivity and a specific porosity correction model. An extended version of the TRANSURANUS fuel performance code including sphere-pac fuel was then developed (D244).

1.3.3 Domain 3

Domain 3 of the F-BRIDGE project had several objectives focused on particle fuel, with potential applications in liquid metal cooled fast reactors as well as gas cooled thermal and fast reactors.

The objectives of domain 3 were achieved through 3 technical work packages.

- WP 3-1: Performance evaluation of advanced sphere-pac fuel options
- WP 3-2: Advanced sphere-pac fuel development and control
- WP 3-3: Assessment of sphere-pac fuel for Generation IV

1.3.3.1 Sphere-pac fuel performance evaluation and assessment for GEN IV (WP3-1 and WP3-3)

F-BRIDGE project has shown the interplay between modelling and technology, drawing on fundamental physics and chemical approaches, coupling them to detailed economic impact analysis and experiment to demonstrate the feasibility of an advanced fuel concept such a sphere-pac.

Sphere-pac fuel as a concept for fast reactor systems has a number of positive attributes, particularly in the area of fabrication. Economic estimates of the cost of a fabrication plant and its operation performed in F-BRIDGE have shown that sphere-pac poses no insurmountable penalties, and the costs are similar to those encountered for pellet fuel fabrication facilities.

Furthermore, a neutronic and a thermal investigation of sphere-pac and advanced concepts with incorporation of an additional phase or replacement of the small particle phase with another material of high thermal conductivity do not introduce a show stopper. The major concern must be the choice of this material. F-BRIDGE evaluations have indicated that Mo is the most favourable of the candidates identified. Others exhibited too low melting point (e.g. Si) or would have to operate above their boiling point (e.g. Na). Fuel bonding with Pb might be a further option to pursue. The F-BRIDGE project successfully demonstrated the feasibility of the consolidation of such advanced options.

The detailed results of WP3-1 and WP3-3 are as follows.

- **Core physics assessment of advanced sphere-pac fuels.** The studies shown that the introduction of sphere-pac fuel is not expected to have adverse effects on the European Sodium Fast Reactor (ESFR) core behaviour, as far as neutronics is concerned (D311).
- **Chemical evaluation of thermally bonded sphere-pac fuel.** The introduction of metallic thermal bond materials is envisaged to improve thermal conductivity of sphere-pac fuels for transmutation of minor actinides in fast reactors. The feasibility of adding these materials, was considered from a chemical perspective and candidates evaluated (D312).
- **Thermal modelling investigation of sphere-pac fuel options.** The (radial) thermal conductivity of sphere-pac fuel was evaluated. The effect of substituting the small sphere fraction in 2-fraction sphere-pac columns by metallic molybdenum and silicon fractions was determined, as well as the effect of substituting the helium bonding gas by liquid metals such as sodium and lead (D313).
- **Evaluation of advanced sphere-pac fuel types.** The results of the evaluation of advanced sphere-pac types based on core physics, thermal, thermomechanical and chemical evaluations of various thermally bonded sphere-pac concepts were presented (D314).
- **Comparison of various fabrication processes and detailed cost evaluation of minor actinide (MA) fuels.** The study considered heterogeneous recycling of exclusively Am and selected the sphere-pac fabrication route as alternative to the standard pellet technology. It compared advanced sol-gel based fabrication technologies to the classical pellet fabrication route derived from the industrial MOX fuel experience (D331).

1.3.3.2 Advanced fuel development and control (WP3-2)

Quality assurance is a key component ensuring the reliability of reactor fuels. The F-BRIDGE project connected advanced experimental methods operating at various size ranges (nm to mm), proving beyond doubt that a basic scientific approach is a key element to underpin quality of nuclear fuels.

Moreover, F- BRIDGE enabled the establishment of a joining technology for an advanced cladding material, with potential gains in the quest for a robust accident tolerant nuclear fuel, by establishing fundamental thermochemical properties of a soldering material to join SiC components.

- **Quality assurance in multiple dimensions:** The F-BRIDGE project provided a unique base for industrial organisations, research centres and universities to establish a systematic procedure to cross validate quality assurance procedures, and in doing so draw on new fundamental scientific methods, operating over size ranges from the nm to mm size ranges. At the upper end of the size range (μm to mm), tomography was successfully applied to the characterisation of an advanced sphere-pac fuel concept. Furthermore, tomography and phase contrast imaging were cross qualified for the determination of dimensions of kernels and coating layers in HTR coated particle fuels. At the nm scale, advanced spectroscopic techniques (Raman and MAS NMR) were developed for the determination of the quality of the layers in coated particle fuels (D321, D327, D329).
- **Joining of ceramic cladding components:** During the course of the F-BRIDGE project, events in Japan indicated that other cladding materials should be investigated to improve accident tolerance of nuclear fuel, and in particular, materials offering a higher margin to melting, and whose interaction with coolant does not result in explosive gas formation. The gas fast reactor is an innovative option that already identified this issue for its high operating temperature regimes. Silicon carbide is a promising material for these applications. Its production is not simple, and indeed a composite of interlinked fibres may well be needed to meet these goals. F-BRIDGE successfully investigated two methods capable of joining SiC tubes and end caps. They were based on a laser soldering method, with the composition of the solder being chosen on the basis of thermodynamic phase diagram calculations. In contrast, electromagnetic pulse technology can be used to weld a metallic collar spanning the joint area (D328, D329). F- BRIDGE enabled the establishment of a joining technology for an advanced cladding material, with potential gains in the quest for a robust accident tolerant nuclear fuel, by establishing fundamental thermochemical properties of a soldering material to join SiC components.

1.3.4 Conclusion

As a conclusion, F-BRIDGE took fully advantage of the use of innovative experimental and modelling techniques combined in a multiscale approach to make significant breakthroughs in the detailed knowledge of the ceramic fuel and cladding behaviour for the performance and safety optimization. The project contributed to produce key basic data and identify relevant mechanisms that are to be used for a better prediction of fuel behaviour. Significant progress has been made in the important objective of F-BRIDGE of linking the various scales of modelling from the atomic to the macroscopic scale. A particular effort has been put in the validation of methods used to improve their reliability. Mesoscopic scale has been identified as a key scale in the multiscale modelling approach since it ensures the concrete connection between data and mechanisms obtained at lower scale to the fuel performance code at macroscopic scale. Regarding the application to advanced fuel design, F-BRIDGE succeeded in assessing the sphere-pac innovative concept and proposing optimized fabrication. It also highlighted how advanced experimental methods can contribute to the quality assurance enabling reliability of reactor fuels. The F-BRIDGE partners contributed effectively to lay the stones joining both end of a bridge between basic research and applied issues, improving knowledge and enabling a better prediction of fuel behaviour and selection of promising fuel systems. Even if a challenge for the future remains that this bridge is used on a routine basis, its construction represents the exceptional success of the F-BRIDGE European project.

1.4 Potential impact, exploitation of results, main dissemination activities

1.4.1 *Potential impact and exploitation of the results*

The F-BRIDGE project corresponded to a strategic need for basic understanding of the behaviour and performance of potential fuel materials to improve fuel design. In this context, the impact from the F-BRIDGE project is as follows:

- **The basis of a long term European cooperation contributing to the European leadership in the field.** Despite its position at the cutting edge of nuclear fuel science and its high level of expertise, the community of European scientists tackling basic research on fuels was small and fragmented at the beginning of the project. At the same time, the scientific competition with other areas in the world was increasing due to the renewed interest in nuclear fission energy worldwide at that time (in particular, but not only, in the United States). F-BRIDGE effectively contributed to strengthen the European cooperation leading so in the increase of the European leadership in this field in a long term perspective. This fruitful cooperation achieved will, however, have to be maintained in the future by new projects.

- **An improved understanding of fuel behaviour under irradiation:** thermodynamic stability, atomic transport phenomena, microstructure evolution and elementary thermo-mechanical properties of candidate fuel materials under the combined effects of high temperature and radiation in service conditions can be used to optimize current fuel regarding performance as well and improved safety and design of future fuels.

- **An improved ability to model fuel materials thanks to basic research and improve and design**

As demonstrated in F-BRIDGE, the accurate and reliable atomistic calculations of fuels materials will allow the assessment of basic material properties. Coupled with experiments, they already contributed, and will contribute even more in the future, to identify relevant mechanisms and to obtain important missing basic data. The mesoscopic scale was identified as a key scale because it bridges data and mechanisms obtained at lower scale to the fuel performance code at macroscopic scale. Multiscale modelling, i.e. the combination of scientifically sound models at the scales of the relevant underlying mechanisms, will contribute to assess the fuel behaviour at the operationally relevant time and length scales.

This modelling effort, which combines theoretical and experimental work, is expected to have a direct impact on the development of innovative fuels. It will provide a scientific basis for the pre-selection of candidate materials. It will contribute in an efficient way to the selection, design and interpretation of the more relevant out of and/or in pile experiments to be done during the licensing process of innovative fuels.

- **The integration of teams and disciplines**

Scientific communities are not just fragmented by their location in Europe, but are also fundamentally fragmented by discipline. Multiscale modelling necessitates the collaboration between all the scientific levels involved, from atomistic modellers, delivering the basic building blocks of understanding, and experimentalists providing essential input and validation data, to end users and performance code developers. This requires that all the people involved look beyond the scope of their normal work.

The F-BRIDGE project was the first integrated project on non-metallic nuclear materials which encompassed all the relevant length and time scales between atomic description and macroscopic systems. Similar investigations had already been performed on irradiation effects in metals in the

framework of the PERFECT (FP6) and PERFORM 60 (FP7) projects, and they significantly improved knowledge in that field.

The successful synergy between the various disciplines involved in F-BRIDGE, which culminated in the development of a multiscale modelling approach of uranium dioxide, enhances the predictive capability of models and contributes to reducing the effort necessary to develop innovative fuels, changing the way nuclear fuel-cladding systems are developed and evaluated. The cooperation between the scientists, engineers and end-users ensures a direct translation of technological issues into basic research investigations, as well as the integration of basic research results into useable qualitative and quantitative information. This will have a significant impact on in-pile behaviour prediction, optimisation of irradiation experiments, innovative fuel design and manufacturing.

Continue the development of such an approach in the future will increase effectiveness and optimal results since the fuel-cladding systems of the future will be based on fundamental understanding of fuel behaviour, which will enable us to determine and optimise the optimal properties for the system under consideration.

- **Recommendations on advanced sphere-pac fuel systems and on ceramic cladding for GEN IV applications**

The challenges faced by Generation IV fuel-cladding systems were addressed by the development and optimisation of particle fuel types based on microspheres fabricated by sol-gel technique and vibratory compacted in a suitable cladding (sphere-pac fuel). The large potential of this fuel type has been recognized for various reactor systems because of their high potential for gas accommodation, reduced fuel/cladding mechanical interaction and favourable manufacturing procedures. It was confirmed in F-BRIDGE that optimized sphere-pac fuels could pave the way to high burn-ups, actinide recycling strategies, as well as proliferation resistant, safe and clean fuel manufacturing processes, which are the key issues to be addressed in Generation IV framework.

Although ceramic claddings such as silicon carbide were mainly envisaged for VHTR and GFR systems, the favourable characteristics of this material can potentially provide increased safety margins for the other Generation IV systems, especially under accidental conditions. By establishing fundamental thermochemical properties of a soldering material to join SiC components, F-BRIDGE enabled the establishment of a joining technology for an advanced cladding material, which may lead to potential gains in the quest for a robust accident tolerant nuclear fuel.

- **Application of the basic research approach to establish a sound scientific and technical basis towards increased safety and competitiveness of existing and future reactors**

Following the 2011 events in Japan, the European Commission decided to put a larger part of its fission research effort to safety issues for the coming years. An essential objective is therefore to establish a sound scientific and technical basis to increased safety and competitiveness of existing and future reactors. Enhanced safety will stem jointly from improvements in understanding of accidents scenarios and through advances in modelling and simulation.

An approach combining basic research and materials science, which has been shown to be a successful and robust one in F-BRIDGE, can be used to establish the scientific basis sought. This approach combined with a top-down analysis of the most critical issues and which should be tackled through basic research, will be able to solve a selection of critical applied issues relating to nuclear fuel behaviour under irradiation in normal and off-normal operating conditions, such as the margin to melting, the control of fission product release and chemistry, the knowledge of microstructural changes and the control of the mechanical integrity. It will yield the missing relevant data and mechanisms underpinning fuel behaviour that will bring about a better understanding, simulation capabilities and hence increased safety.

As a conclusion the joint efforts done in F-BRIDGE on basic research in nuclear fuel science, as well as transfer and integration of its results and recommendations on innovative ceramic composite fuels such as sphere-pac, are of high relevance to improve the efficiency of present fuels and to assess the potential of advanced reactor systems such as those considered in the Generation IV International Forum. The basic research approach developed and the results obtained in F-BRIDGE will contribute to increase the safety of nuclear reactors. It will also help explore the potential of more advanced technology to deliver an even safer, more resource efficient and more competitive exploitation of nuclear energy.

1.4.2 Dissemination of F-BRIDGE results

The valorisation of F-BRIDGE activities leaned on standard tools, such as an internet web site (www.f-bridge.eu), a brochure presenting the project distributed at events, the presentation of the project in the EC FP7 booklet, as well as a newsletter.

F-BRIDGE has put a significant effort in the dissemination and valorisation of the results of the investigation performed. This has led to approximately 80 peer-reviewed articles published in scientific literature and to 60 comprehensive project deliverables, from which 34 public ones are already available for the international community.

The synthesis of F-BRIDGE results were presented to the European and international community at the final international workshop of the project organized in February 2012. The program of this workshop included presentations of the main results obtained in F-BRIDGE, external invited talks presenting research related to F-BRIDGE activities and a poster session for PhD students and post doctorate associates involved in F-BRIDGE, giving them the opportunity to present their results to the international community. The workshop was a success with more than 80 participants including F-BRIDGE participants and researchers from the European and international fuel communities. Many countries were represented: France, UK, Germany, The Netherlands, Sweden, Switzerland, Belgium, and Latvia, but also the US and Japan. The international scientific advisory committee members and the European industry representatives from the user group also attended the international workshop.

F-BRIDGE coordinator and participants were very active in participating in the most important international conferences in the nuclear material field, in particular the Nuclear Material conference (NuMat), meetings of the Materials research society (MRS), the Materials Modelling and Simulation of Nuclear Fuel workshop series (MMSNF), where the status of the project and scientific results were regularly presented. F-BRIDGE supported the organization of NuMat 2010 in Germany and MMSNF 2011 in France. F-BRIDGE coordination was involved in the co-organization of the “Material Challenges in Current and Future Nuclear Technologies” symposium of the 2011 MRS fall meeting. In addition, F-BRIDGE was cited and participants interviewed in an article from “Chemical and Engineering News” journal on “Nuclear Efficiency: with new fuel formulation, reactors could extract more energy and reduce hazardous waste” in 2010.

Several F-BRIDGE partners were also representatives or key contributors to the OECD/NEA working party on multiscale modelling of nuclear fuels and materials, promoting so the European research and increasing the international cooperation. Regarding fuels, the objective of this working party is to promote the multiscale modelling of fuel by producing two state-of-the-art reports. The first one focuses on the modelling of the relevant phenomena involved in fuel behaviour and of fuel properties, while the second one presents the validation of modelling methods and approximations used at the atomic scale.

At the European level, F-BRIDGE project was presented at several SNETP general assemblies (2008, 2010, and 2011), as well as at the 2009 FISA conference. F-BRIDGE also had close relationships with other European projects (CP-ESFR, PERFORM 60, GETMAT, ACTINET I3,...) thanks to common participants, mutual attendance of plenary meetings and exchange of deliverables. F-BRIDGE coordinator was moreover part of the ACTINET I3 scientific advisory committee.

A particular success of F-BRIDGE is the fruitful interaction with European industry representatives from the user group which allowed the construction of a list of key technological issues that basic research can

contribute to solve. This interaction contributed to the good dissemination of the F-BRIDGE results to European industry.

F-BRIDGE also had the opportunity to communicate with the European civil community through an interview of the coordinator and project participants for a report on European research on nuclear issues of the TV show “L’Europe dans tous ses états” of the French channel “Public Sénat”.

Regarding education and training activities, two successful schools were organized during the project and contributed to strengthen the links between senior scientists and students: the first one was dedicated to “Ceramic nuclear fuel and cladding materials” and the second one to “the synergy between modelling and experiments for the investigation of nuclear fuels and materials under irradiation”. Participation of more than 40 students in each school, including overseas participants, and the very positive feedback from participants were a clear proof that F-BRIDGE met its objective of dissemination thanks to training.

Finally, another proof of the high quality of the work performed in F-BRIDGE was the attractiveness to young scientists proved by the large number of PhD students and post doctorate associates - 34 -, involved in the project. A real success of F-BRIDGE is that most of these students have been hired in European companies or research organizations.

1.5 Public web site and contact information



Website address: www.f-bridge.eu

Project type: Collaborative Project (Small- or Medium-Scaled Focused Research Project)

Project start date: 01/03/2008

Duration: 48 months

Total budget: EUR 10,201,705

EC contribution: EUR 5,450,000

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2 Use and dissemination of foreground

2.1 Scientific publications

No	Title	Main author	Title of periodical or series	Number, date or frequency	Year of publication	Relevant pages	Permanent identifier	Open access
1	Basic research in support of innovative fuels design for the GEn IV systems: The F-BRIDGE project	C. Valot	Nucl. Eng. Des.	241	2011	3521	http://dx.doi.org/10.1016/j.nucengdes.2011.08.021	No
2	Irradiation effects in helium implanted silicon carbide measured by X-ray absorption spectrometry	M. A. Pouchon	J. Nucl. Mater.	385	2009	299	http://dx.doi.org/10.1016/j.jnucmat.2008.12.017	No
3	Impact of auto-irradiation on the thermophysical properties of oxide nuclear reactor fuels	D. Staicu	J. Nucl. Mater.	397	2010	8	http://dx.doi.org/10.1016/j.jnucmat.2009.11.024	No
4	Oxygen diffusion in relation to p-type doping in uranium dioxide	P. Garcia	J. Nucl. Mater.	400	2010	112	http://dx.doi.org/10.1016/j.jnucmat.2010.02.019	No
5	Helium release in uranium dioxide in relation to grain boundaries and free surfaces	G. Martin	Nucl. Instrum. Methods B	268	2010	2133	http://dx.doi.org/10.1016/j.nimb.2010.02.064	No
6	Irradiation-induced heterogeneous nucleation in uranium dioxide	G. Martin	Phys. Lett. A	374	2010	3038	http://dx.doi.org/10.1016/j.physleta.2010.05.033	No
8	Silver Diffusion in Coated Fuel Particles	E. Lopez-Honorato	J. Am. Ceram. Soc.	93	2010	3076	http://dx.doi.org/10.1111/j.1551-2916.2010.04055.x	No
9	Effect of microstructure on the resilience of silicon carbide to Palladium attack	E. Lopez-Honorato	J. Am. Ceram. Soc.	93	2010	4135	http://dx.doi.org/10.1111/j.1551-2916.2010.04005.x	No
10	Silver diffusion in SiC coatings	E. Lopez-Honorato	J. Am. Ceram. Soc.	94	2011	3064	http://dx.doi.org/10.1111/j.1551-2916.2011.04544.x	No

11	An in situ TEM study of the evolution of Xe bubble populations in UO ₂	A. Michel	Nucl. Instrum. Methods B	272	2012	218	http://dx.doi.org/10.1016/j.nimb.2011.01.069	No
12	Irradiation damage effects on helium migration in sintered uranium dioxide	G. Martin	Nucl. Instrum. Methods B	273	2012	122	http://dx.doi.org/10.1016/j.nimb.2011.07.055	No
13	Nucleation and growth of intragranular defect and insoluble atom clusters in nuclear oxide fuels	P. Garcia	Nucl. Instrum. Methods B	277	2012	98	http://dx.doi.org/10.1016/j.nimb.2011.12.031	No
14	A study of helium mobility in polycrystalline uranium dioxide ,	P. Garcia	J. Nucl. Mater.	430	2012	156	http://dx.doi.org/10.1016/j.jnucmat.2012.06.001	No
15	A TEM study of bubbles growth with temperature in xenon and krypton implanted uranium dioxide	A. Michel	Defect Diffus. Forum	323-325	2012	191	http://dx.doi.org/10.4028/www.scientific.net/DDF.323-325.191	No
16	Iodine volume diffusion measurements in uranium dioxide	E. Pizzi	Defect Diffus. Forum	323-325	2012	197	http://dx.doi.org/10.4028/www.scientific.net/DDF.323-325.197	No
17	Elaboration of uranium monocarbide samples for diffusion studies	O. Fiquet	Defect Diffus. Forum	323-325	2012	253	http://dx.doi.org/10.4028/www.scientific.net/DDF.323-325.253	No
18	Chemisorption of a molecular oxygen on the UN(001) surface: Ab initio calculations	Yu.F. Zhukovskii	J. Nucl. Mater.	393	2009	504	http://dx.doi.org/10.1016/j.jnucmat.2009.07.010	No
19	First principles calculations of oxygen adsorption on the UN (001) surface	Yu.F. Zhukovskii	Surface Science	603	2009	50	http://dx.doi.org/10.1016/j.susc.2008.10.019	No
20	First-principles study of uranium carbide: Accommodation of point defects and of helium, xenon, and oxygen impurities	M. Freyss	Phys. Rev. B	81	2010	014101	http://dx.doi.org/10.1103/PhysRevB.81.014101	No
21	Density functional theory calculations on magnetic properties of actinide compounds	D. Gryaznov	Phys. Chem. Chem. Phys.	12	2010	12273	http://dx.doi.org/10.1039/C0CP00372G	No
22	DFT calculations of point defects on UN(001) surface	D. Bocharov	Surf. Sci.	605	2011	396	http://dx.doi.org/10.1016/j.susc.2010.11.007	No

23	<i>Ab initio</i> modeling of oxygen impurity atom incorporation into uranium mononitride surface and sub-surface vacancies	D. Bocharov	J. Nucl. Mater.	416	2011	200	http://dx.doi.org/10.1016/j.jnucmat.2010.11.090	No
24	Ab initio modelling of volatile fission products in Uranium mononitride	M. Klipfel	J. Nucl. Mater.	422	2012	137	http://dx.doi.org/10.1016/j.jnucmat.2011.12.018	No
25	First principles simulations on surface properties and oxidation of nitride nuclear fuels (not present in SESAM report)	D. Bocharov	Advances in Nuclear Fuel	1 book	2012	Ch. 5	http://dx.doi.org/10.5772/1917	Yes
26	The first-principles treatment of the electron-correlation and spin-orbital effects in uranium mononitride nuclear fuels	D. Gryaznov	Phys. Chem. Chem. Phys.	14	2012	4482	http://dx.doi.org/10.1039/c2cp40297a	No
27	Laser melting of uranium carbides	C.A. Utton	J. Nucl. Mater.	385	2009	443	http://dx.doi.org/10.1016/j.jnucmat.2008.12.031	No
28	Reassessing the melting temperature of PuO ₂	F. De Bruycker	Mater. Today	13	2010	52	http://dx.doi.org/10.1016/S1369-7021(10)70204-2	No
29	Mass spectrometric studies of the vapor phase in the Pu-O system	P. Gotcu-Freis	J. Chem. Thermodyn.	43	2011	1164	http://dx.doi.org/10.1016/j.jct.2011.02.024	No
30	The melting behaviour of plutonium dioxide: a laser heating study	F. De Bruycker	J. Nucl. Mater.	416	2011	166	http://dx.doi.org/10.1016/j.jnucmat.2010.11.030	No
31	Thermodynamic modelling of advanced oxide and carbide nuclear fuels: Description of the U–Pu–O–C systems	C. Guéneau	J. Nucl. Mater.	419	2011	145	http://dx.doi.org/10.1016/j.jnucmat.2011.07.033	No
32	On the melting of uranium/plutonium mixed dioxides with high-Pu content: A laser heating study	F. De Bruycker	J. Nucl. Mater.	419	2011	186	http://dx.doi.org/10.1016/j.jnucmat.2011.08.028	No
33	Modeling multiple defects in ionic phases like UO _{2±x} using the Compound Energy Formalism	B. Sundman	Acta Mater.	59	2011	6039	http://dx.doi.org/10.1016/j.actamat.2011.06.012	No
34	The melting behaviour of oxide nuclear fuels: effects of the oxygen potential studied by laser heating	D. Manara	Procedia Chem.	7	2012	505	http://dx.doi.org/10.1016/j.proche.2012.10.077	No

35	Ionization energies for the actinide mono- and dioxides series, from Th to Cm: theory versus experiment	I. Infante	J. Phys. Chem. A	114	2010	6007	http://dx.doi.org/10.1021/jp1016328	No
36	How accurate are electronic structure methods for actinide chemistry?	B. Averkiev	Theor. Chem. Acc.	129	2011	657	http://dx.doi.org/10.1007/s00214-011-0913-0	No
37	A thermodynamic study of the Pu-Am-O system	P. Gotcu-Freis	J. Nucl. Mater.	414	2011	408	http://dx.doi.org/10.1016/j.jnucmat.2011.05.014	No
38	(Solid+gas) equilibrium studies for neptunium dioxide	P. Gotcu-Freis	J. Chem. Thermodyn.	43	2011	492	http://dx.doi.org/10.1016/j.jct.2010.10.027	No
39	The vaporisation behaviour of americium dioxide by use of mass spectrometry	P. Gotcu-Freis	J. Nucl. Mater.	409	2011	194	http://dx.doi.org/10.1016/j.jnucmat.2010.12.024	No
40	Computed vibrational frequencies of actinide oxides $AnO^{0/+2+}$ and $AnO_2^{0/+2+}$ (An = Th, Pa, U, Np, Pu, Am, Cm)	A. Kovács	J. Phys. Chem. A	115	2011	6646	http://dx.doi.org/10.1021/jp202538k	No
41	Theoretical study of the structure and bonding in ThC_2 and UC_2	P. Pogány	J. Phys. Chem. A	116	2012	747	http://dx.doi.org/10.1021/jp210190m	No
42	Theoretical study of bond distances and dissociation energies of actinide oxides AnO and AnO_2	A. Kovács	Inorg. Chem	51	2012	4841	http://dx.doi.org/10.1021/ic300275y	No
43	Theoretical study of the Pu and Am dicarbide molecules	P. Pogány	Struct. Chem.	23	2012	1281	http://dx.doi.org/10.1007/s11224-012-0075-2	No
44	A molecular dynamics study of radiation induced diffusion in uranium dioxide	G. Martin	J. Nucl. Mater.	385	2009	351	http://dx.doi.org/10.1016/j.jnucmat.2008.12.010	No
45	GGA+U study of the incorporation of iodine in uranium dioxide	B. Dorado	Eur. Phys. J. B	69	2009	203	http://dx.doi.org/10.1140/epjb/e2009-00145-0	No
46	DFT+U calculations of the ground state and metastable states of uranium dioxide	B. Dorado	Phys. Rev. B	79	2009	235125	http://dx.doi.org/10.1103/PhysRevB.79.235125	No
47	Computer simulation of defects formation and equilibrium in non-stoichiometric uranium dioxide	E. Yakub	J. Nucl. Mater.	389	2009	119	http://dx.doi.org/10.1016/j.jnucmat.2009.01.029	No
48	Predicting the probability for fission gas resolution into uranium dioxide	D.C. Parfitt	J. Nucl. Mater.	392	2009	28	http://dx.doi.org/10.1016/j.jnucmat.2009.03.046	No

49	Self-diffusion near symmetrical tilt grain boundaries in UO ₂ matrix: a molecular dynamics simulation study	E. Vincent-Aublant	J. Nucl. Mater.	392	2009	114	http://dx.doi.org/10.1016/j.jnucmat.2009.03.059	No
50	Large molecular dynamics simulations of collision cascades in mono-crystal, bicrystal, and poly-crystal UO ₂	L. Van Brutzel	Nucl. Instr. Methods B	267	2009	3013	http://dx.doi.org/10.1016/j.nimb.2009.06.078	No
51	Molecular dynamics simulation of helium and oxygen diffusion in UO _{2+x}	K. Govers	J. Nucl. Mater.	395	2009	131	http://dx.doi.org/10.1016/j.jnucmat.2009.10.043	No
52	An atomistic approach to self-diffusion in uranium dioxide	B. Dorado	J. Nucl. Mater.	400	2010	103	http://dx.doi.org/10.1016/j.jnucmat.2010.02.017	No
53	Strain field and line energies of dislocations in uranium dioxide	D.C. Parfitt	J. Phys.: Condens. Matt.	22	2010	175004	http://dx.doi.org/10.1088/0953-8984/22/17/175004	No
54	Atomistic study of stability of xenon nanoclusters in uranium oxide	A. Chartier	Phys. Rev. B	81	2010	174111	http://dx.doi.org/10.1103/PhysRevB.81.174111	No
55	Stability of oxygen point defects in UO ₂ by first-principles DFT+U calculations: importance of occupation matrix control and Jahn-Teller distortion	B. Dorado	Phys. Rev. B	82	2010	035114	http://dx.doi.org/10.1103/PhysRevB.82.035114	No
56	On the solution and migration of single Xe atoms in uranium dioxide – An interatomic potentials study	K. Govers	J. Nucl. Mater.	405	2010	252	http://dx.doi.org/10.1016/j.jnucmat.2010.08.013	No
57	Establishing the isotropy of displacement cascades in UO ₂ through molecular dynamics simulation	C.L. Bishop	Nucl. Inst. Meth. B	268	2010	2915	http://dx.doi.org/10.1016/j.nimb.2010.05.007	No
58	Comment on “Interplay of defect cluster and the stability of xenon in uranium dioxide from density functional calculations”	B. Dorado	Phys. Rev. B	84	2011	096101	http://dx.doi.org/10.1103/PhysRevB.84.096101	No
59	Effect of the cascade energy on defect production in uranium dioxide	G. Martin	Nucl. Instrum. Methods B	269	2011	1727	http://dx.doi.org/10.1016/j.nimb.2010.12.075	No

60	Segregation of xenon to dislocations and grain boundaries in uranium dioxide	P.V. Nerikar	Phys. Rev. B	84	2011	174105	http://dx.doi.org/10.1103/PhysRevB.84.174105	No
61	First-principles calculation and experimental study of oxygen diffusion in uranium dioxide	B. Dorado	Phys. Rev. B	83	2011	035126	http://dx.doi.org/10.1103/PhysRevB.83.035126	No
62	Solution of trivalent cations into uranium dioxide	S.C. Middleburgh	J. Nucl. Mater.	420	2012	258	http://dx.doi.org/10.1016/j.jnucmat.2011.10.006	No
63	Assessment of density functional theory for bonds formed between rare gases and open-shell atoms: computational study of small molecules containing He, Kr and Xe	M. Bertolus	Phys. Chem. Chem. Phys.	14	2012	553	http://dx.doi.org/10.1039/c1cp22324k	No
64	Molecular dynamics study of Xe bubble re-resolution in UO ₂	K. Govers	J. Nucl. Mater.	420	2012	282	http://dx.doi.org/10.1016/j.jnucmat.2011.10.010	No
65	The influence of dipole polarisation on threshold displacement energies in UO ₂	C.L. Bishop	Nucl. Instrum. Meth. B	274	2012	195	http://dx.doi.org/10.1016/j.nimb.2011.11.023	No
66	Modelling Fission Gas Bubble Distribution in UO ₂	R. Skorek	Defect Diffus. Forum	323-325	2012	209	http://dx.doi.org/10.4028/www.scientific.net/DDF.323-325.209	No
67	Molecular dynamics study of grain boundary diffusion of fission gas in uranium dioxide	K. Govers	Defect Diffus. Forum	323-325	2012	215	http://dx.doi.org/10.4028/www.scientific.net/DDF.323-325.215	No
68	Free energy of Xe incorporation at point defects, in nanovoids and bubbles in UO ₂	S. Murphy	Phys. Rev. B	85	2012	144102	http://dx.doi.org/10.1103/PhysRevB.85.144102	No
69	First-principles calculations of uranium diffusion in uranium dioxide	B. Dorado	Phys. Rev. B	86	2012	035110	http://dx.doi.org/10.1103/PhysRevB.86.035110	No
70	Atomistic Simulation of Nuclear Fuels (not present in SESAM report)	M. Krack	MRS Symp. Proc.	1383	2012	19	http://dx.doi.org/10.1557/opl.2012.520	No
71	Frenkel pair recombinations in UO ₂ : Importance of explicit description of polarizability in core-shell molecular dynamics simulations	F. Devynck	Phys. Rev. B	85	2012	184103	http://dx.doi.org/10.1103/PhysRevB.85.184103	No

72	Multiscale modelling exercise on the transport properties of uranium dioxide under irradiation (not present in SESAM report)	M. Bertolus	J. Nucl. Mater.				Submitted in April 2013	No
73	Implementing first principles calculations of defect migration in a fuel performance code for UN simulations	E.A. Kotomin	J. Nucl. Mater.	393	2009	292	http://dx.doi.org/10.1016/j.jnucmat.2009.06.016	No
74	Modeling and simulation of nuclear fuel materials	R. Devanathan	Energy Environ. Sci	3	2010	1406	http://dx.doi.org/10.1039/C0EE00028K	No
75	Multiscale modelling for the fission gas behaviour in the TRANSURANUS code	P. Van Uffelen	Nucl. Eng. Technol.	43	2011	477	http://dx.doi.org/10.5516/NET.2011.43.6.477	No
76	Characterization of the anisotropy of PyC by Raman spectroscopy	E. López-Honorato	Carbon	48	2010	881	http://dx.doi.org/10.1016/j.carbon.2009.11.010	No
77	Analysis of the anisotropy, stoichiometry and polytypes in pyrolytic carbon and silicon carbide coatings	E. López-Honorato	J. Nucl. Mater.	432	2013	334	http://dx.doi.org/10.1016/j.jnucmat.2012.08.030	No
78	Silicon carbide polytype characterisation in coated fuel particles by Raman spectroscopy and ^{29}Si magic angle spinning NMR	E. López-Honorato	J. Nucl. Mater.	433	2013	199	http://dx.doi.org/10.1016/j.jnucmat.2012.08.047	No

Table 1: List of scientific peer reviewed publications

2.2 Dissemination activities

No	Type of activities	Main leader	Title	Date	Place	Type of audience	Size of audience	Countries addressed
1	Web	B. Duplantier	Public web site	May 2008	www.f-bridge.eu	Scientific Community, Industry, Civil Society	~ 3000 visitors per year	International -World
2	Interview	C. Valot	Interview of the coordinator and project participants for a report on European research on nuclear issues for the show “L'Europe dans tous ses états”	01/05/2008	French TV channel “Public Sénat”	Civil Society, Policy makers		France
3	Presentation	C. Valot	Oral communication: presentation of the project	September 2008	MMSNF workshop, Karlsruhe, Germany	Scientific Community		International -World
4	Presentation	C. Valot	Presentation of the project for the OECD/NSC working party on multiscale modelling on nuclear materials and fuels (WPMM)	September 2008	OECD/NEA, Issy-les-Moulineaux, France	Scientific Community		International -World
5	Poster	V. Chauvet	Poster: presentation of the project	November 2008	SNETP General Assembly, Brussels, Belgium	Scientific Community, Industry, Policy makers		International - Europe
6	Flyer	M. Bertolus	Presentation of the project for EC FP7 booklet	December 2008	European Commission	Scientific Community, Industry, Policy makers		International - Europe

7	Presentation	C. Valot	Oral communication: general presentation of F-BRIDGE	06/2009	FISA 2009, Prague, The Czech Republic	Scientific Community, Policy makers	International - Europe
8	Presentation	C. Valot	Oral presentation of the project at the ATR NSU user week	06/2009	Idaho Falls, USA	Scientific Community	International - World
9	Flyer	B. Duplantier	F-BRIDGE brochure to be distributed at events	06/2010	Distributed	Scientific Community	1000 flyers distributed International - World
10	Poster	J. Somers	Poster: presentation of the progress made in the project	09/2010	SNETP General Assembly, Brussels, Belgium	Scientific Community, Industry, Policy makers	International - Europe
11	Article published in the popular press	M. Bertolus	Interview of F-BRIDGE participants for the article on “Nuclear efficiency: with new fuel formulation, reactors could extract more energy and reduce hazardous waste” by Jyllian N. Kemsley	09/2010	Chemical & Engineering News	Scientific Community Civil Society	International - World
12	Thesis	B. Dorado	Etude des propriétés de transport atomique dans le dioxyde d'uranium par le calcul de structure électronique : influence des fortes corrélations	15/09/2010	Cadarache, France	Scientific Community	International - Europe
13	Summer school	P. Van Uffelen	First F-BRIDGE School on “Ceramic nuclear fuel and cladding materials”	28/09/2010-02/10/2010	Karlsruhe, Germany	Scientific Community	International - World
14	Conference	C. Valot	Support to the first Nuclear Materials Conference	10/2010	Karlsruhe, Germany	Scientific Community	International - World
15	Thesis	F. De Bruycker	High temperature phase transitions in nuclear fuels of the fourth generation	10/12/2010	Orléans, France	Scientific Community	International -Europe
16	Flyer	B. Duplantier	F-BRIDGE newsletter	03/2011	Various events	Scientific Community	International - Europe
17	Thesis	P. Gotcu-Freis	High temperature thermodynamic studies on the transuranium oxides and their solid solutions	15/06/2011	Delft, The Netherlands	Scientific Community	International -Europe

18	Summer school	I. Farnan	Second F-BRIDGE School on “Synergy between modelling and experiments for the investigation of nuclear fuels and materials under irradiation”	19/09/2011-23/09/2011	Cambridge, UK	Scientific Community	International - World
19	Workshop	C. Valot	Co-organization of the 2011 MMSNF workshop, as well as financial support from the project	26/09/2011-28/09/2011	Aix-en-Provence, France	Scientific community	International - World
20	Presentation	B. Duplantier	Poster: presentation of the progress made in the project	11/2011	SNETP General Assembly, Brussels, Belgium	Scientific Community, Policy makers	International - Europe
21	Conference	M. Bertolus	Co-organization of the “Material Challenges in Current and Future Nuclear Technologies” symposium of the 2011 MRS fall meeting	12/2011	Boston, USA	Scientific community	International - World
22	Thesis	A. Michel	Etude du comportement des gaz rares dans le dioxyde d'uranium : mécanismes de diffusion, nucléation et grossissement des bulles	13/12/2011	Cadarache, France	Scientific community	France
23	Workshop	C. Valot	Final international workshop	23/02/2012	Aix en Provence, France	Scientific community	International - World
24	Thesis	P. Fossati	Contribution à l'étude des propriétés mécaniques du combustible nucléaire : Modélisation atomistique de la déformation du dioxyde d'uranium	20/11/2012	Ecole Centrale Paris, France	Scientific community	France
25	Thesis	T. Belhabib	Comportement thermique des défauts lacunaires induits par l'hélium et les gaz de fission dans le dioxyde d'uranium	18/12/2012	Orléans, France	Scientific community	France

Table 2: List of dissemination activities

2.3 Exploitable foreground

The exploitable foreground includes:

- Peer-reviewed articles published in scientific literature (see section 2.1)
- PhD theses (see section 2.2)
- Public deliverables, which are available on the F-BRIDGE public website (www.f-bridge.eu) and are therefore accessible to the whole scientific community.
- Confidential deliverables, which can be obtained by parties external to the project, provided all owners agree to make it available to this party. Therefore, if an author is asked by an external party to provide a copy of a deliverable, this author should ask for the authorization of all the partners involved in the deliverable. Until February 28th 2015, i.e. 3 years after the end of the project, the author should also inform the coordinator.

The list of public and confidential deliverables given below contains experimental and/or calculation results, assessment, recommendations.

Type of Exploitable Foreground	Description of exploitable foreground	Confidential	Foreseen embargo date	Exploitable product(s) or measure(s)	Sector(s) of application	Timetable, commercial or any other use	Patents or other IPR exploitation	Owner & Other Beneficiary(s) involved
General advancement of knowledge	Experimental investigations of irradiation induced diffusion of He and I in UO ₂	No		Reports Experimental data	M72 - Scientific research and development	Available on public web site starting March 2013, Contribution of Euratom to GIF	N/A	CEA, CNRS (owners)
General advancement of knowledge	Experiments on the thermal diffusion of oxygen in UO ₂	No		Report Experimental data	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CEA, CNRS (owners)
General advancement of knowledge	Effect of auto-radiation damage on the specific heat and thermal diffusivity of (U,Pu)O ₂ and UO ₂	No		Report Experimental data	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	JRC-ITU (owner)
General advancement of knowledge	Diffusion of ³⁷ Cl in UO ₂ with FP irradiation at high energy	No		Report Experimental data	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CNRS (owner)

Type of Exploitable Foreground	Description of exploitable foreground	Confidential	Foreseen embargo date	Exploitable product(s) or measure(s)	Sector(s) of application	Timetable, commercial or any other use	Patents or other IPR exploitation	Owner & Other Beneficiary(s) involved
General advancement of knowledge	Fabrication and first characterisations of uranium carbide samples	No		Report Experimental data	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CEA, CNRS (<i>owners</i>)
General advancement of knowledge	Microstructure of Irradiated SiC: interfaces in SiC/SiC composites, point defects and amorphisation in crystalline SiC and influence of the dimensionality	No		Report Experimental data	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	UCAM, UMAN, JRC-ITU, PSI, NRG, ANP-F, (<i>owners</i>)
General advancement of knowledge	Investigation of Ag diffusion in SiC	No		Report Experimental data	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	UMAN (<i>owner</i>)
General advancement of knowledge	Behaviour of defects, fission products and oxygen and the effect of non-stoichiometry in bulk UN and (U,Zr)N	No		Report Calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	JRC-ITU, ISSP, IMPERIAL (<i>owners</i>)
General advancement of knowledge	Behaviour of defects, fission products and oxygen and effect of non-stoichiometry in bulk actinide carbides	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CEA, MD (<i>owners</i>)
General advancement of knowledge	Electronic structure investigation of the behaviour of defects and oxygen impurities at the uranium nitride surface	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	ISSP (<i>owner</i>)
General advancement of knowledge	Atomic scale modelling of the effects of irradiation and diffusion near SiC grain boundaries	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013	N/A	PSI (<i>owner</i>)
General advancement of knowledge	Pair interaction model for U-Pu-O and U-Pu-C: Ab initio calculations of model parameters	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CEA (<i>owner</i>)

Type of Exploitable Foreground	Description of exploitable foreground	Confidential	Foreseen embargo date	Exploitable product(s) or measure(s)	Sector(s) of application	Timetable, commercial or any other use	Patents or other IPR exploitation	Owner & Other Beneficiary(s) involved
General advancement of knowledge	Report on the experimental work on U-Pu-O	No		Reports experimental data	M72 - Scientific research and development	Available on public web site starting March 2013	N/A	JRC-ITU, CEA (<i>owners</i>)
General advancement of knowledge	Updated phase diagram of the U-C system	No		Report experimental and calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CNRS, JRC-ITU, CT, CEA (<i>owners</i>)
General advancement of knowledge	Thermodynamic modelling of the U-Pu-O-C system using the Calphad method	No		Reports calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CEA, CT, JRC-ITU (<i>owners</i>)
General advancement of knowledge	Experimental results on the (U-Pu-C-O) system	No		Report experimental and calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	JRC-ITU, CEA, CT, CNRS (<i>owners</i>)
General advancement of knowledge	Preparation, characterization, melting behaviour of Selected Grey Phase Compounds	No		Reports Experimental data	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	NRG (<i>owner</i>)
General advancement of knowledge	<i>Ab initio</i> modelling of molecular actinide compounds	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	BME, JRC-ITU (<i>owners</i>)
General advancement of knowledge	Americium and plutonium chemistry in MOX fuel: X-ray diffraction and X-ray absorption spectroscopy characterization	No		Report experimental data	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CEA (<i>owner</i>)
General advancement of knowledge	Thermodynamic modelling of the U-Pu-Am-Np-O system	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CEA, JRC-ITU, CT (<i>owners</i>)

Type of Exploitable Foreground	Description of exploitable foreground	Confidential	Foreseen embargo date	Exploitable product(s) or measure(s)	Sector(s) of application	Timetable, commercial or any other use	Patents or other IPR exploitation	Owner & Other Beneficiary(s) involved
General advancement of knowledge	Results on the U-Mo-C system	No		Report experimental data	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CNRS, JRC-ITU, (<i>owners</i>)
General advancement of knowledge	Experimental determination and thermodynamic modelling of the U-Pu-Si-C system	No		Reports experimental and calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CNRS, CEA (<i>owners</i>)
General advancement of knowledge	Development and assessment of atomistic modelling methods for the investigation of fuel materials under operational conditions	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013, Contribution of Euratom to GIF	N/A	CEA, IMPERIAL, PSI, SCK-CEN (<i>owners</i>)
General advancement of knowledge	Investigation using atomic scale methods of the transport properties of bulk UO ₂ containing defects and fission products	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	JRC-ITU, CEA, IMPERIAL, PSI, SCK-CEN (<i>owners</i>)
General advancement of knowledge	Empirical potential investigation of transport properties in polycrystalline UO ₂ and in the presence of extended defects	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	IMPERIAL, CEA, SCK-CEN (<i>owners</i>)
General advancement of knowledge	Thermo-mechanical properties of complex microstructures	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	IMPERIAL, CEA, (<i>owners</i>)
General advancement of knowledge	Application of mesoscale approaches to the diffusion processes in bulk and near extended defects	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CEA, (<i>owner</i>)

Type of Exploitable Foreground	Description of exploitable foreground	Confidential	Foreseen embargo date	Exploitable product(s) or measure(s)	Sector(s) of application	Timetable, commercial or any other use	Patents or other IPR exploitation	Owner & Other Beneficiary(s) involved
General advancement of knowledge	Multiscale exercise on transport properties in uranium dioxide	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CEA, IMPERIAL, JRC-ITU, PSI, SCK-CEN (<i>owners</i>)
General advancement of knowledge	Key material properties and behaviour for modelling input and validation purposes	No		Report calculation results	M72 - Scientific research and development	Available on public web site starting March 2013; Contribution of Euratom to GIF	N/A	CEA, NRG (<i>owners</i>)
General advancement of knowledge	Data request lists attaching industrial issues to scientific effort requirements	YES		Report List of data	M72 - Scientific research and development	Use by project partners starting February 2012; External use submitted to owners' authorization	N/A	CEA, NRG, JRC-ITU (<i>owners</i>)
General advancement of knowledge	Lessons learned from the past experiments on advanced fuels	YES		Report Experiments, recommendations	M72 - Scientific research and development	Use by project partners starting April 2011; External use submitted to owners' authorization; Contribution of Euratom to GIF starting April 2012	N/A	JRC-ITU (<i>owner</i>)
General advancement of knowledge	EBSD measurements on irradiated UO ₂	YES		Report Experimental data	M72 - Scientific research and development	Use by project partners starting July 2012; External use submitted to owners' authorization	N/A	NRG (<i>owner</i>)

Type of Exploitable Foreground	Description of exploitable foreground	Confidential	Foreseen embargo date	Exploitable product(s) or measure(s)	Sector(s) of application	Timetable, commercial or any other use	Patents or other IPR exploitation	Owner & Other Beneficiary(s) involved
General advancement of knowledge	Identification and general description of dedicated irradiation tests and PIE to effectively contribute to multiscale modelling efforts	YES		Report Recommendations	M72 - Scientific research and development	Use by project partners starting July 2012; External use submitted to owners' authorization; Contribution of Euratom to GIF starting July 2013	N/A	NRG (<i>owner</i>)
General advancement of knowledge	Functionalities of the SPHERE and SPACON codes	YES		Report Code Documentation	M72 - Scientific research and development	Use by project partners starting January 2011; External use submitted to owners' authorization	N/A	PSI (<i>owner</i>)
General advancement of knowledge	Material properties for nitride and carbide fuels	YES		Report Material properties	M72 - Scientific research and development	Use by project partners starting April 2011; External use submitted to owners' authorization	N/A	JRC-ITU, CEA (<i>owners</i>)
General advancement of knowledge	Implementation of material properties in the TRANSURANUS fuel performance code	YES		Report New code version	M72 - Scientific research and development	Use by project partners starting February 2012; External use submitted to owners' authorization	N/A	JRC-ITU, NRG (<i>owners</i>)
General advancement of knowledge	Implementation of new models in the new version of the TRANSURANUS fuel performance code	YES		Report New code version	M72 - Scientific research and development	Use by project partners starting August 2012; External use submitted to owners' authorization	N/A	NRG (<i>owner</i>)
General advancement of knowledge	Advanced sphere-pac fuels: a core physics assessment	YES		Report Concept assessment	M72 - Scientific research and development	Use by project partners starting December 2012; External use submitted to owners' authorization; Contribution of Euratom to GIF starting December 2013	N/A	NRG, FZJ (<i>owners</i>)

Type of Exploitable Foreground	Description of exploitable foreground	Confidential	Foreseen embargo date	Exploitable product(s) or measure(s)	Sector(s) of application	Timetable, commercial or any other use	Patents or other IPR exploitation	Owner & Other Beneficiary(s) involved
General advancement of knowledge	Chemical Evaluation of Thermally Bonded Sphere-Pac Fuel	YES		Report Concept assessment	M72 - Scientific research and development	Use by project partners starting March 2012; External use submitted to owners' authorization; Contribution of Euratom to GIF starting March 2013	N/A	NRG (<i>owner</i>)
General advancement of knowledge	Thermal conductivity of sphere-pac columns containing thermal bond materials	YES		Report Concept assessment	M72 - Scientific research and development	Use by project partners starting March 2012; External use submitted to owners' authorization; Contribution of Euratom to GIF starting March 2013	N/A	NRG (<i>owner</i>)
General advancement of knowledge	Evaluation of Advanced Sphere-pac fuel types	YES		Report Concept assessment	M72 - Scientific research and development	Use by project partners starting August 2012; External use submitted to owners' authorization	N/A	NRG (<i>owner</i>)
General advancement of knowledge	Advanced Sphere-pac Manufacturing: Progress and Achievements	YES		Review on Manufacturing process	M72 - Scientific research and development	Use by project partners starting March 2012; External use submitted to owners' authorization; Contribution of Euratom to GIF starting March 2013	N/A	JRC-ITU (<i>owner</i>)

Type of Exploitable Foreground	Description of exploitable foreground	Confidential	Foreseen embargo date	Exploitable product(s) or measure(s)	Sector(s) of application	Timetable, commercial or any other use	Patents or other IPR exploitation	Owner & Other Beneficiary(s) involved
General advancement of knowledge	Joining of ceramics and performance characterization	YES		Report, Technical assessment	M72 - Scientific research and development	Use by project partners starting April 2012; External use submitted to owners' authorization, Contribution of Euratom to GIF starting April 2013	N/A	TUD, JRC-ITU (<i>owners</i>)
General advancement of knowledge	Advanced fuel development and control	YES		Report, Concept assessment	M72 - Scientific research and development	Use by project partners starting July 2012; External use submitted to owners' authorization	N/A	JRC-ITU, UMAN, UCAM, ANP-F, TUD (<i>owners</i>)
General advancement of knowledge	Fabrication data for (U,Am)O ₂ fuels	YES		Report, Technical and economical concept assessment	M72 - Scientific research and development	Use by project partners starting April 2012; External use submitted to owners' authorization, Contribution of Euratom to GIF starting April 2013	N/A	FEX (<i>owner</i>)

Table 3: List of exploitable foreground

3 Societal implications

B. Ethics

1. Did your project undergo an Ethics Review (and/or Screening)? **NO**

If Yes: have you described the progress of compliance with the relevant Ethics Review/Screening Requirements in the frame of the periodic/final project reports?

2. Please indicate whether your project involved any of the following issues:

RESEARCH ON HUMANS

- Did the project involve children? **NO**
- Did the project involve patients? **NO**
- Did the project involve persons not able to give consent? **NO**
- Did the project involve adult healthy volunteers? **NO**
- Did the project involve Human genetic material? **NO**
- Did the project involve Human biological samples? **NO**
- Did the project involve Human data collection? **NO**

RESEARCH ON HUMAN EMBRYO/FOETUS

- Did the project involve Human Embryos? **NO**
- Did the project involve Human Foetal Tissue / Cells? **NO**
- Did the project involve Human Embryonic Stem Cells (hESCs)? **NO**
- Did the project on human Embryonic Stem Cells involve cells in culture? **NO**
- Did the project on human Embryonic Stem Cells involve the derivation of cells from Embryos? **NO**

PRIVACY

- Did the project involve processing of genetic information or personal data (eg. health, sexual lifestyle, ethnicity, political opinion, religious or philosophical conviction)? **NO**
- Did the project involve tracking the location or observation of people? **NO**

RESEARCH ON ANIMALS

- Did the project involve research on animals? **NO**
- Were those animals transgenic small laboratory animals? **NO**
- Were those animals transgenic farm animals? **NO**
- Were those animals cloned farm animals? **NO**
- Were those animals non-human primates? **NO**

RESEARCH INVOLVING DEVELOPING COUNTRIES

- Did the project involve the use of local resources (genetic, animal, plant etc)? **NO**
- Was the project of benefit to local community (capacity building, access to healthcare, education etc)? **NO**

DUAL USE

- Research having direct military use **NO**
- Research having the potential for terrorist abuse **NO**

C. Workforce Statistics

3. Workforce statistics for the project: Please indicate in the table below the number of people who worked on the project (on a headcount basis).

Type of Position	Number of Women	Number of Men
Scientific Coordinator	2	0
Work package leaders	5	8
Experienced researchers (i.e. PhD holders)	19	45
PhD Students	7	15
Other		

4. How many additional researchers (in companies and universities) were recruited specifically for this project? **10**

Of which, indicate the number of men: **7**

D. Gender Aspects

5. Did you carry out specific Gender Equality Actions under the project? Yes No

6. Which of the following actions did you carry out and how effective were they?

	Not at all effective	Very effective
<input type="checkbox"/> Design and implement an equal opportunity policy	<input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/>	<input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/>
<input type="checkbox"/> Set targets to achieve a gender balance in the workforce	<input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/>	<input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/>
<input type="checkbox"/> Organise conferences and workshops on gender	<input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/>	<input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/>
<input type="checkbox"/> Actions to improve work-life balance	<input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/>	<input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/> <input type="radio"/>
<input type="radio"/> Other:		

7. Was there a gender dimension associated with the research content – i.e. wherever people were the focus of the research as, for example, consumers, users, patients or in trials, was the issue of gender considered and addressed?

- Yes- please specify
- No

E Synergies with Science Education

8. Did your project involve working with students and/or school pupils (e.g. open days, participation in science festivals and events, prizes/competitions or joint projects)?

Yes- please specify

2 summer schools organized for students
Coordinator presented project to high school students during science days

No

9. Did the project generate any science education material (e.g. kits, websites, explanatory booklets, DVDs)?

Yes- please specify

No

H Use and dissemination

14. How many articles were published / accepted for publication in peer-reviewed journals? 74

To how many of these is open access provided? 1

How many of these are published in open access journals? 1

How many of these are published in open repositories?

To how many of these is open access not provided? 73

Please check all applicable reasons for not providing open access:

- publisher's licensing agreement would not permit publishing in a repository
- no suitable repository available
- no suitable open access journal available
- no funds available to publish in an open access journal
- lack of time and resources
- lack of information on open access
- other, (for instance: classification for security project):

15. How many new patent applications ('priority filings') have been made? 0
 ("Technologically unique": multiple applications for the same invention in different jurisdictions should be counted as just one application of grant).

16. Indicate how many of the following Intellectual Property Rights were applied for (give number in each box).

Trademark	0
Registered design	0
Other	0

17. How many spin-off companies were created / are planned as a direct result of the project? 0

Indicate the approximate number of additional jobs in these companies:

18. Please indicate whether your project has a potential impact on employment, in comparison with the situation before your project:

- | | |
|---|--|
| <input type="checkbox"/> Increase in employment, or | <input type="checkbox"/> In small & medium-sized enterprises |
| <input checked="" type="checkbox"/> Safeguard employment, or | <input checked="" type="checkbox"/> In large companies |
| <input type="checkbox"/> Decrease in employment, | <input type="checkbox"/> None of the above / not relevant to the project |
| <input type="checkbox"/> Difficult to estimate / not possible to quantify | |

19. For your project partnership please estimate the employment effect resulting directly from your participation in Full Time Equivalent (FTE = one person working fulltime for a year) jobs: *Indicate figure:*

Difficult to estimate / not possible to quantify ✓

I Media and Communication to the general public

20. As part of the project, were any of the beneficiaries professionals in communication or media relations?

Yes No

21. As part of the project, have any beneficiaries received professional media / communication training / advice to improve communication with the general public?

Yes No

22 Which of the following have been used to communicate information about your project to the general public, or have resulted from your project?

- | | |
|---|--|
| <input type="checkbox"/> Press Release | <input checked="" type="checkbox"/> Coverage in specialist press |
| <input type="checkbox"/> Media briefing | <input type="checkbox"/> Coverage in general (non-specialist) press |
| <input checked="" type="checkbox"/> TV coverage / report | <input type="checkbox"/> Coverage in national press |
| <input type="checkbox"/> Radio coverage / report | <input type="checkbox"/> Coverage in international press |
| <input checked="" type="checkbox"/> Brochures /posters / flyers | <input checked="" type="checkbox"/> Website for the general public / internet |
| <input type="checkbox"/> DVD /Film /Multimedia | <input type="checkbox"/> Event targeting general public (festival, conference, exhibition, science café) |
-

23 In which languages are the information products for the general public produced?

- | | |
|--|---|
| <input type="checkbox"/> Language of the coordinator | <input checked="" type="checkbox"/> English |
| <input type="checkbox"/> Other language(s) | |
-

Table 4: Societal and socio-economic issues addressed by the project

4 Annex - Document approval by authors' organisations

#	Name of beneficiary	Approved by	Function	Date
1	Commissariat à l'Energie Atomique	Françoise Touboul	GB member	?
2	AREVA NP SAS	Pierre Guillemier	GB member	?
3	CalculThermo	Nathalie Dupin	GB member	?
4	Centre National de la Recherche Scientifique	Catherine Bessada	GB member	?
6	Nuclear Fuel Experts SA	Hubert Bairiot	GB member	?
7	Forschungszentrum Jülich	Rahim Nabbi	GB member	?
8	Budapest University of Technology and Economics	Attila Kovacs	GB member	?
9	Imperial College of Science, Technology and Medicine	Robin Grimes	GB member	?
10	Institute of Solid State Physics	Eugen Kotomin	GB member	?
11	Joint Research Centre (Institute for Transuranium Elements)	Rudy Konings	GB member	?
12	LGI Consulting	Vincent Chauvet	GB member	?
13	LISTO bvba	Luc Van Den Durpel	GB member	?
14	Materials Design	Alexander Mavromaras	GB member	?
15	Nuclear Research & consultancy Group	Sander de Groot	GB member	?
16	Paul Scherrer Institut	Martin Zimmermann	GB member	?
17	Studiecentrum voor Kernenergie - Centre d'Etude de l'Energie Nucléaire	Marc Verweft	GB member	?
18	Universität Dresden	Wolfgang Lippman	GB member	?
19	University of Cambridge	Ian Farnan	GB member	?
20	University of Manchester	Ping Xiao	GB member	?