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Analysis of Options and Experimental Examination of Fuels for Water Cooled Reactors with Increased Accident Tolerance (ACTOF)

Final Report of a Coordinated Research Project

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ANNEX

COUNTRY REPORTS FROM PARTICIPANTS

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A STARTING POINT OF THE ASSESSMENT OF ACCIDENT TOLERANT FUELS

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Abstract

The 2011 accident in Fukushima improves the need for enhanced alloys and/or materials for Fuel Elements (FFEE) to be more tolerant to mistakes as developed in the design bases of Nuclear Power Plant (NPP), including Loss of Coolant Accident (LOCA) and other severe accidents. These difficulties also include the use as carriers of fissile isotopes of other FFEE materials and design. Without abandoning the ideas of assembly of cylindrical pipes and each fuel rod as a tube or sheath containing cylindrical pellets, these objectives should be accomplished. In essence, other ideas such as distributed or spherical fuels are not excluded because licensing can be much harder and more costly. The initiative called "Accident Tolerant Fuels" (ATF) arises from these demands, the problems of which can also be utilized by designs of Gen IV (Generation IV International Forum). The closure of the Halden Reactor Project and the lack of sufficient irradiation equipment forced us to enhance the modelling of fuel to meet the information demands for the suggested fresh components and designs of fuel. In order to finish the ambitious agenda for nuclear energy improvements, international collaboration is compulsory.

1. PROPOSAL OF THE CNEA WORKING GROUP

We initiate diverse lines of work by taking into account the response in our institution (CNEA and Instituto Balseiro-UNCuyo). The work was focussed in two aspects. One of both was the promotion of the safety issues of the ATF materials and design in the nuclear forums, companies and utilities of our country as the presentation of these studies in several national meetings of science and nuclear technology. The second is preparation of the new nuclear engineers by a complete inclusion of these topics in our courses of materials and fuels.

Those lines of investigation and developments were as follows:

- Headlines about material properties;
- Modelling:
  - by using M³:
    - SiC;
  - by using BFS:
    - FeCrAl;
- FeCrAl elemental development in order to validate modelling:
  - Experimental support of the theoretical calculation;
  - Theoretical calculation support of the experimental and technical procedures;
- BaCo code:
  - Onset of validation of new materials with BaCo;
  - Simulations;
- “Blind test”, a CRP ACTOF code intercomparison:
  - BaCo results for the comparison proposal;
  - A preview of BaCo3D calculations for different fuel materials;

— Neutronic evaluation of ATF:
  - A basic ATF CANDU fuel proposal;
  - Economic overview.

Several CNEA groups were summoned with an academic point of view due to our scarce experience in these materials for NPPs (“Nuclear Power Plants”). Nevertheless, we have experience with MOX fuels and it were initiated some UN developments. A better position we have for MTR ("Material Testing Reactor" or experimental reactors) fuels in particular with the use of AlU, U_3O_8, SiC and UMo.

2. MATERIAL PROPERTIES

The databases available for UO_2 and Zr alloys contain accurate data on the components used in present fuel element designs. A distinct scenario occurs when considering, under standard conditions, under irradiation conditions and after irradiation, the material characteristics of potential Accident Tolerant Fuels (ATF) elements.

2.1. Fuel Materials

Considering the material of nuclear fuel, the primary objectives are: (1) improve thermal conductivity resulting in reduced fuel pellet working temperature; (2) improve dimensional stability that could be obtained by producing stable porosity that would accommodate gaseous products that would reduce the release of these gasses to the plenum, (3) improve the U density to reduce enrichment. There is some precious experience gained in the operation of MTR and naval reactors for the choice of fuel components. Dispersed fuels are the ones best suited to the conservative elements needed in a BC's design.

From the performance and integrity point of view of fuel elements (FF.EE.), those related to heat transfer and mechanical behaviour are the most relevant properties. If the resistance to corrosion and oxidation is improved, heat and hydrogen generation would be reduced, thereby improving FF.EE tolerance in serious accidents. This strategy aims to reinforce aspects that significantly delay the onset of failure or those that initiate an advanced accidental stage. UO_2 compares unfavourably with UC and metallic U from the point of view of thermal conductivity [1]. UO_2's greater melting point offsets this disadvantage (see Table 2.4. of Ref. [1], p. 34).

2.2. Cladding Materials

During the 2011 Fukushima accident, under the extreme circumstances induced by that event, weak performance of present fuel elements based on UO_2/Zry was found. For this reason, a considerable boost has been given to the design of fuel elements tolerant to accidents or ATF. This initiative involves the creation of fresh fuel element ideas, materials and designs that would make them more resistant to the environmental circumstances associated with severe accidents. One particular requirement is that they must tolerate long-term loss of cooling scenarios (LOCA), without affecting the performance of the fuel elements during the nuclear power plant's normal operation. Probably the most significant element in developing a new ATF is the choice of materials. The following options stand out in view of possible cladding materials:

— Regular Zr-based alloys cladding protected by external coating (Cr, Ni Cr, Ti, SiC, ZrN);
— Cladding based on steel (ferritic, austenitic, steel, etc.) where the accumulated FBR and naval reactor knowledge could be helpful;
— High alloy steel, particularly FeCrAl (commercially referred to as "Kanthal");
— SiC ceramic cladding (or SiC composite combinations);
— Mo-based alloys.

These clad materials exhibit greater resistance to corrosion than Zry. However, it would affect the neutron economy. Therefore, consideration should be given to a rise in enrichment that compensates for neutron loss.

2.3. Physical properties

On the one side, the most important features are connected to heat transfer and mechanical properties, take into account the efficiency of the fuel elements. On the other side, taking into account the tolerance to major accidents, the importance switches to improve corrosion and oxidation resistance, limiting, among others, heat and hydrogen generation. That is, the primary objective is to reinforce elements that considerably delay the onset of failure or prevent those that would cause an advanced accidental phase.

Phenomena such as plasticity, creep and irradiation growth are highly interrelated and, moreover, are highly non-linear. For each of these physical events, particular models need to be defined. These models should be compatible at the same time. Extensive technical and experimental data on steels is available [2]. Also, well documented are the various Zr-based alloys used by the nuclear industry.

SiC is a ceramic material. It displays a high resistance to creep and no plasticity; particularly in the temperature ranges of interest [3−5] (see Table 3 of Ref [3], p. 1202). However, this material can be produced by different methods, which result in a broad range of variation in their physical and thermomechanical properties. There is an acceptable amount of information about solid SiC in the literature. Considering possible nuclear applications, it possesses a remarkably low creep rate at temperatures of interest. A SiC/SiC type cladding has been proposed which in essence is a solid SiC tube covered by SiC fibers. Solid SiC and SiC fibers present different properties and mechanical behaviour, a characteristic that complicates the formulation of models for the component. Among the set of possible metallic alloys proposed as cladding materials, FeCrAl stands out. There is abundant information about the basic properties of this material [1]. However, it is important to remember that phenomena and properties should be modelled under nuclear fuel irradiation conditions. The comparative analysis of the properties of some of those materials can guide us on the issues of safety and behaviour in order to design an ATF. Ref. [4] includes a review of some basic fuel material parameters as linear thermal expansion coefficient (α) of Zry, SiC (see Ref. [6]) and FeCrAl as a function of temperature, thermal conductivity (k), Young's -elastic-modulus, Poisson's ratio among others. The values obtained from the literature present a wide disparity and even errors in some cases. A possible explanation is that the materials considered are not yet standardized for nuclear use. Their basic characteristics are not well specified (impurities, anisotropy-isotropy, crystalline structure, grain size, manufacturing route, etc.).

3. M³ METHODOLOGY APPLIED TO ATF NUCLEAR MATERIALS

3.1. Introduction

A relevant stage in the development of ATF fuels is the need of new models and simulation codes of its behaviour under normal conditions and under irradiation together with advanced calculation techniques and computational tools that effectively assist the design of conventional fuels, new Advanced Tolerant Fuels (ATF) designs and materials for Generation-IV reactors.

The scarce experimental information of the proposed new materials can be complemented with first principles or ab initio calculations that enable a deep theoretical support comparable to the one usually intended for experimental support, producing an authentic synergy between experiments and theoretical models. The disadvantage of these studies is the absence of reliable data in comparison with the current available database for UO_2 and Zr alloys. The methodology of Multi-Scale Modelling of Materials ("M³") was proposed as a way to partially fill the gap between the empirical codes and the needs of new materials data.

3.2. Multiscale Modelling of Materials – M³

The detailed understanding of the atomic and electronic structures and defect mobility under various conditions requires a multiscale modelling approach. As consequence, there is a great need to complement the available experimental and phenomenological methods by means of atomistic (nano-scale) techniques such as molecular dynamics (MD) and kinetic Monte Carlo (KMC), in combination with first-principles calculations. Since the availability and accuracy of the inter-atomic potentials, including those for multi-component compounds, represents a major issue for the application of atomistic techniques such as MD or KMC, it is essential to compare the results among various techniques and experiments for self-consistency and validation. Moreover, molecular dynamics simulations require an intensive use of powerful computers and therefore the inter-atomic potentials to be used must be computationally efficient as well as physically appropriate for the description of the properties of the fuels and materials to be used in the ATF and Generation IV reactors.

There has been a considerable interest in actinide nitrides and carbides [7, 8] during the last years due to the Generation-IV reactor initiative and at present for the development of ATF. In order to predict fuel performance under different operating conditions and to understand the evolution of a spent fuel over long period of time, it is necessary to develop a better experimental and theoretical knowledge of the defect induced processes and the accumulation of fission products. In view of this prospect, the knowledge of the physical and thermal properties of carbides and nitrides is of crucial importance for modelling the fuel behaviour. The current experimental database could be enough to support empirical correlations and modelling for current fuels. Nevertheless, new

approaches are required if the actual fuel computer codes will be used to simulate ultra high burn up and in particular if new materials and extreme situations will be included in future research programs. M³ is a new field in Computational Material Science that allows the study of complex phenomena such the behaviour of new fuels and cladding materials, and as consequence, could provide a theoretical methodology to obtain the required information. The M³ methodology is based on the electronic structure calculations through ab initio codes and allow the study of structural, electronic and elastic properties at T = 0 K. Also it is possible to obtain properties at finite temperature through phonon calculations. The methodology is followed by the development of effective or model potentials, whose parameters can be determined by using experimental data, to be used in MD and KMC codes [8, 9]. However, the application of the molecular dynamics simulations to obtain a detailed description, from an atomistic point of view, of the diffusion mechanism and transport properties requires an intensive use of powerful computers. Indeed, the dynamic structure must be simulated over considerably long time steps and therefore the inter-atomic potentials used must be computationally efficient as well as physically appropriate for the description of the properties of the fuels and materials to be used in the ATF designs and the Generation IV reactors.

An overview of methods, algorithm, software and keywords of M³ (see Figure 1):

- Ab initio methods:
  - Density Functional Theory ("DFT");
- Ab initio methods II:
  - all electrons:
    - LAPW (Linearized Augmented Planewave) [code Wien2k];
    - LMTO (Linear Muffin-Tin Orbital) [code Stuttgart];
    - Gaussians (code Crystal);
  - Pseudopotentials:
    - Plane Waves (codes VASP/Q-Espresso/Abinit);
    - Local Orbitals (code Siesta);
- Molecular Dynamic ("MD");
- Monte Carlo Algorithms:
  - Metropolis Monte Carlo;
  - Kinetics Monte Carlo ("KMC").

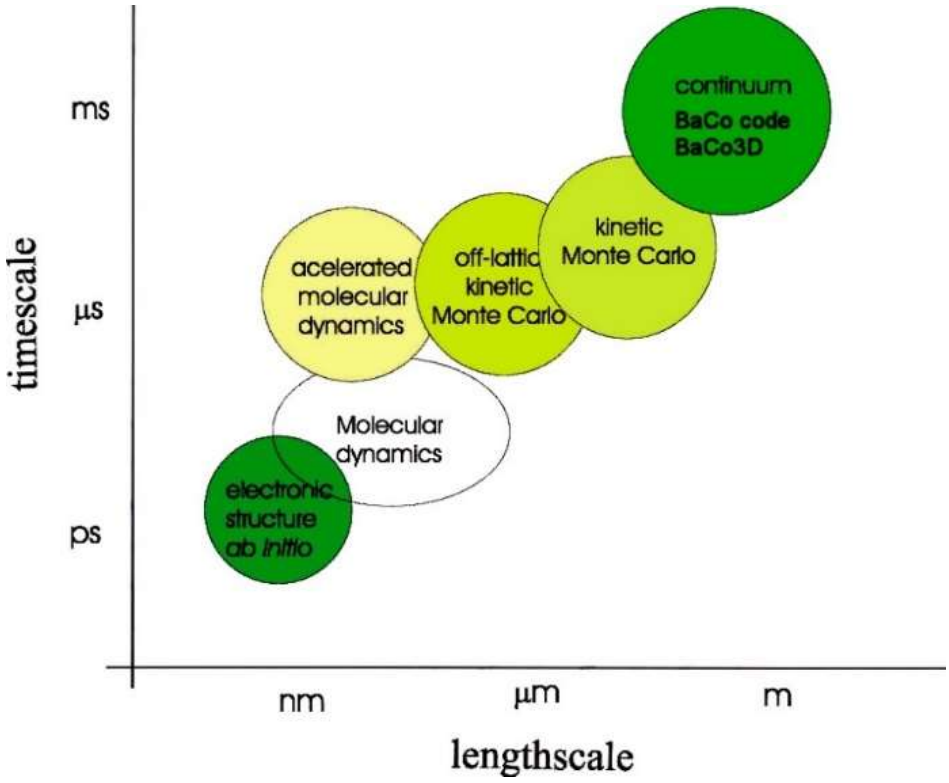

FIG. 1. Different methodologies and experimental techniques into a simplified Time-Length Scales showing the fields of application of each it.

3.3. Toward the Multiscale Modelling of ATF and GEN-IV Reactors – *fcc Th*

The findings of an alternative methodology are provided in Ref. [10] where a free parameter pair potential is implemented to describe the mechanical and thermal properties of *fcc Th* (based on theoretical rather than experimental information).

The ab initio phonon dispersion calculations represent a considerable advance in the understanding of the Th properties from a theoretical point of view [11]. The thermal equation of state and thermodynamic properties such as heat capacity, thermal pressure and entropy can be obtained. Also, the properties of *Th* under high temperature and high pressure were calculated. The elastic constants were calculated using two different approaches. The calculated the elastic constants, lattice parameter, bulk modulus, elastic constants and related material properties were summarized in the Table 1 of Ref. [10] including a comparison with experimental data [12] and previous theoretical results computed from the phonon spectrum and *ab initio* calculations [12, 13]. Based on the calculated elastic constants and by using a quasi-harmonic approximation we have been able to study the thermodynamic properties of *Th* such as thermal expansion coefficient, Grüneisen parameters and Debye temperature finding results with a good accuracy. The results were also presented in Table 1 of Ref. [10]. It is noteworthy the agreement between the result of that reference with the experimental and previous theoretical ones based on phonon calculations.

ThC represents an example of the limitation found in the research of new fuel and materials due to the limited experimental information available. Table 2 of Ref. [14] shows available information from *ab initio* calculations of lattice parameter, bulk modulus and elastic constant for *ThC* phase β1.

The nature of the outcomes described in such works indicates that modelling has reached the point where it is possible to obtain efficient and practical responses, becoming a source of unavailable experimental data on present appropriate issues in ATF and/or Generation IV frameworks.

3.4. M³ Methods, Discussion and Comments

In addition to benchmarking against accessible databases, theoretical research using *ab initio* computing codes is essential to predict the thermo-mechanical characteristics of new fuel structures and/or cladding materials. Material parameters extracted from M³ are included in the BaCo code structure to integrate these ATF components in preliminary evaluation simulations. The data collected so far is promising and helpful for future designs of fuels that are more tolerant to accidental situations.

Nowadays, the need for new material parameters could be addressed through the use of M³ to include new products and extend the modelling and code field of implementation. Actinides carbide and nitride are examples of the limitations observed in researching fresh fuel and equipment owing to the restricted accessible experimental data. The findings presented in this study suggest that modelling has reached the point where it is possible to obtain efficient and practical responses, becoming a source of experimental data to present appropriate issues in ATF and Generation IV frameworks.

4. M³ METHODOLOGY APPLIED TO β-SiC

Silicon carbide is described as a big family of "polytypical" crystalline structures. This manifests this compound's capacity to crystallize in countless changes which can be defined as distinct stacking sequences of the same unit layer. Ref. [15] describes and analyses the calculations of the elastic constants and the thermal properties of the β-SiC in particular the Young's modulus, the specific heat and the linear thermal expansion coefficient. In view of its possible future use in ATF and the accessibility of published references, we decided to begin studying the SiC β-phase as a first step. Ref. [15] shows a good agreement with other authors. The findings achieved for the structural parameters and the elastic constants (based on DFT) are consistent with prior calculations [15, 16]. This would show that *ab-initio* calculations can provide a foundation for modelling more complicated materials (graphens, fibers, etc.) that can be used to forecast their structural and elastic properties independently of experiments. The M³ strategy has become a strong instrument to obtain the information currently absent. M³ synergistically offers powerful assistance for the innovation of nuclear fuel products as shown in the case of cladding *SiC* and *FeCrAl*. The basic calculations show a good agreement with the present data. The significance of minimizing pellet-cladding interactions when using solid *SiC* cladding is an especially appropriate consequence.

5. M³ METHODOLOGY APPLIED TO FeCrAl

5.1. Introduction

Theoretical and modelling calculations of nuclear fuels and their interactions with cladding are limited due to the large number of elements to be considered and the impact that this has on the ability of traditional methods to deal with them. Even when applicable, the development of potentials and parameters needed constitutes a nearly insurmountable obstacle due to the sheer number of interactions to be considered and the ensuing computational demands on even the simplest calculations. Quantum approximate methods are therefore ideal for this task, providing useful information without the need of extensive calculations. In particular, the particular approach on which the BFS method is built facilitates the study of very complex systems. Based on perturbation theory and with a proven degree of accuracy relative to ab initio calculations, the BFS method does not have any formal limitation in terms of how many and what elements may be considered, keeping the same level of accuracy for any arbitrary combination of elements. This property was largely proven in previous applications of BFS to nuclear fuels [17–21] and high entropy alloys [22–25]. In addition, the methodology has no restrictions in terms of the symmetries embedded in the system, equally dealing with bulk and surfaces with the same level of accuracy and computational work.

5.2. BFS applications in nuclear materials

The earliest application of BFS to UZr [17] highlights the additional benefits of using quantum approximate methods. The system is particularly simple (a γU–βZr) solid solution), but by being able to transition from bulk to surface, the study was able to explain fine effects leading to the favourable segregation of Zr to the surface and the structure of the near-surface region, in itself the first step in the proper description of any fuel/cladding interaction problem. In this case, the study explained the reasons why the Zr protective barrier forms near the surface, how it does so preferably for UZr fuel with low Zr concentration, and how it sets the groundwork to understand how the inclusion of other alloying additions in the fuel or the presence of fission products could alter the fine balance needed to minimize the fuel/cladding interaction.

This fundamental study of UZr was followed by an exhaustive study of the formation of lanthanide-rich precipitates in U-Zr fuel and the strong migration patterns to the fuel surface, reacting with cladding elements [18]. This pattern of rapid migration which occurs even at very low burnup was previously understood in terms of a model of vapour phase transport, by which lanthanides migrate through a network of interconnected porosity creating a pathway to the surface. However, this model hardly accounted for the remarkable quantity of these elements near or at the fuel/cladding interface nor does it explains the intricate properties of the resulting surface. The BFS study was done on a complex 7-element system: $U_{70}Zr_{20}Ce_2Pr_2Nd_2Pm_2Sm_2$ and provided an explanation for the strong migration patterns as a function of temperature. Whether the surface is the outer surface of the fuel or a pore in its bulk, the calculation explained the low temperature regime characterized by the depletion of Zr in the subsurface due primarily to Ce segregation, an intermediate temperature regime where Zr repopulates the subsurface region in addition to all the other present lanthanides, and a high temperature regime with stronger Zr segregation and lanthanide-driven surface reconstruction. Exceedingly low values of the lanthanide surface energy were identified as the driving force for the observed behaviour, primarily for the case of Ce, together with the interplay between the surface energies and other elemental properties for different surface orientations.

A subsequent study [19] dealt with the problem of lanthanide migration to the fuel surface by identifying potential candidates for additions to the fuel (In, Ga, Tl) for immobilization of lanthanides, in a way to prevent the formation of a lanthanide-rich surface, which may strongly interact with the cladding. This line of work concluded with the analysis of other elements (Ga, Sb, Pd) [20] as possible lanthanide immobilizers, and Sb and Pd were determined to be the most effective additions, by properly balancing their ability to bind lanthanides in the fuel with their own segregating tendencies. While Sb has lower surface energy than Pd, the BFS study of the 8-element system UZrSbZrLn (Ln = Ce, Pr, Nd, Pm, Sm) shows that precipitates survive to higher temperatures, thus maximizing the ability of Sb to trap Ln in the fuel bulk. Pd is nearly equally effective, but mostly due to its very high surface energy, which precludes Ln segregation to the outer layers of the fuel. The calculations helped identify a specific range for the ratio between the additive and the present Ln for maximizing the Ln immobilization effect (0.7 to 1.4), which constitutes a useful guideline for the inclusion of additives being that the fissioning of nuclear fuel continually adds to the amount of fission-product lanthanide inventory.

The next step was to examine the interaction of UZr with FeNiCr cladding [21], identifying interesting features regarding the interaction of cladding elements and the UZr surface. The simple concepts of BFS strain

and chemical energy helped to explain the experimental observation of HT9 cladding with U-Zr and interdiffusion of Fe, Cr and Ni.

In addition to the study of nuclear fuels, the BFS method was also applied to the novel and interesting case of high-entropy alloys (HEA), systems with a nearly equiatomic distribution of n elements (n > 5). Nearly all identified HEAs form homogeneous solid solutions and exhibit, as a consequence, very interesting properties, not seen in traditional binary- or ternary-based alloys. For the case of solid nuclear fuels, which may well be considered as HEAs due to the large number of elements, it is important to note that the self-healing properties of HEAs (local melting and recrystallization due to thermal spikes) makes them excellent candidates for some nuclear applications. Once again, the excessive number of elements that form HEAs precludes traditional theoretical or modelling methods from providing insight on their behaviour and properties but, once again, the simple formulation of the BFS method and its ability to equally deal with small or large number of elements constitutes an important tool for examining such systems. Several recent applications of BFS to HEAs [22-25] offer evidence that the methodology could be of help in understanding subtle effects in such complex systems, thus expanding the ability to model diverse nuclear fuels of increasing complexity.

For past and future applications of BFS to the nuclear problem, an extensive database of BFS parameters is already available, including all lanthanides, actinides, and most fuel elements. The needed parameters includes single-element bulk properties (cohesive energy, lattice parameter, bulk modulus) and, for every possible pair of elements, their respective BFS perturbative parameters (ΔAB, ΔBA). Because these parameters are obtained from the single crystals and binary combinations, they are straightforwardly computed using ab initio methods. The current database includes U, Pu, Zr, In, Ga, Tl, Sb, Pd, Sn, Te, Be, Al, Mo, Bi, Fe, Ni, Cr, C, La, Ce, Pr, Nd, Pm, Sm, Th, Pa, Np, Am, and Cm, as well as their binary combinations. It should be noted that no additional input is needed for the study of multicomponent systems.

5.3. BFS method for alloys

"As it was mentioned, the BFS method is a quantum approximate method suitable for applications to multicomponent systems [18, 22]. The method is based on the notion that the energy of formation of a given atomic configuration (with unrestricted number and type of elements) can be defined as the superposition of the individual atomic contributions,$\Delta \mathrm{H} = \Sigma\varepsilon_{\mathrm{i}}\ \Delta H = \sum \varepsilon_i$. Each individual contribution $\varepsilon_{\mathrm{i}}\varepsilon_i$consists of a strain energy term, $\varepsilon_i^S\varepsilon_{\mathrm{i}}^{\mathrm{S}}$, which accounts for the change in geometry relative to a single monoatomic crystal of the reference atom i, and a chemical energy term, $\varepsilon_i^C\varepsilon_{\mathrm{i}}^{\mathrm{C}}$, where every neighbour of the reference atom i is in an equilibrium lattice site of a crystal of species ***i***, but retaining their chemical identity. To completely separate the effect of changes in geometry (strain energy) from changes in chemical composition (chemical energy), a reference term, $\varepsilon_i^{C_0}\varepsilon_{\mathrm{i}}^{\mathrm{C_0}}$, is added in the calculation of the chemical energy, computed in the same way as ε_i^C , but where the neighbours of the reference atom have the same identity as the reference atom. A coupling function, g_i, ensures the correct volume dependence of the chemical energy contribution (i.e. the chemical energy vanishes at large interatomic distances). The net contribution $\varepsilon_{\mathrm{i}}\varepsilon_i$to the total energy of formation is then" [25]

$$\varepsilon_{\mathrm{i}} = \varepsilon_{\mathrm{i}}^{\mathrm{S}} + \mathrm{g_i}\left(\varepsilon_{\mathrm{i}}^{\mathrm{C}}\text{-}\varepsilon_{\mathrm{i}}^{\mathrm{C_0}}\right)\varepsilon_i = \varepsilon_i^s + g_i\left(\varepsilon_i^c - \varepsilon_i^{c_0}\right) \quad (1)$$

5.4. BFS in FeCrAl

"The parameters needed for the calculation of the different contributions are easily determined using the Linearized Augmented Plane Wave method [26]. The single element parameters (for Fe, Al, and Cr) are obtained from the zero temperature equation of state of the pure bcc solids, while the interaction parameters needed for the calculation of the chemical energy are obtained from the energy of formation as a function of volume curves for each and every one of the bcc-based binary combinations of all the elements. A full description of the steps needed to compute the different terms in Eq. 1 can be found in Ref. [27]. Finally, temperature effects are obtained from large scale Monte Carlo simulations, described in detail in Ref. [22]. Previous relevant applications of the BFS method to nuclear fuels can be found in Refs. [18, 21, 28]. BFS was used in order to obtain basic material parameters as the "linear thermal expansion coefficient", specific heat, Bulk modulus and others (see Figs 2 – 4)" [25]

It was sketched the BFS method as a powerful tool in order to obtain the parameters of materials used in the new design of ATF and the Gen-IV initiative. We are incorporating the results in the BaCo code.

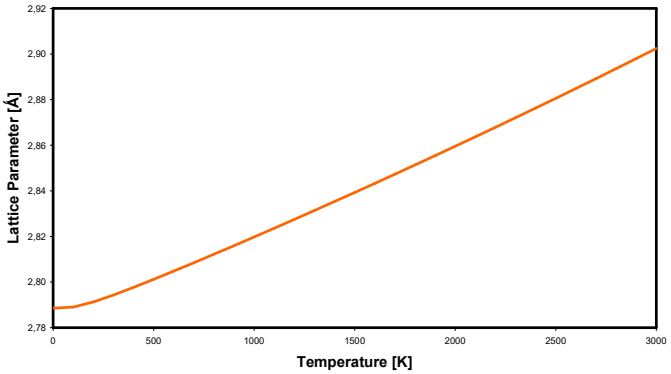

FIG. 2. Lattice parameter of FeCrAl calculated with BFS.

$A = -9\times10^{-13}\ T^3 + 6\times10^{-9}\ T^2 + 3\times10^{-5}\ T + 2.786$, *A in Å.*

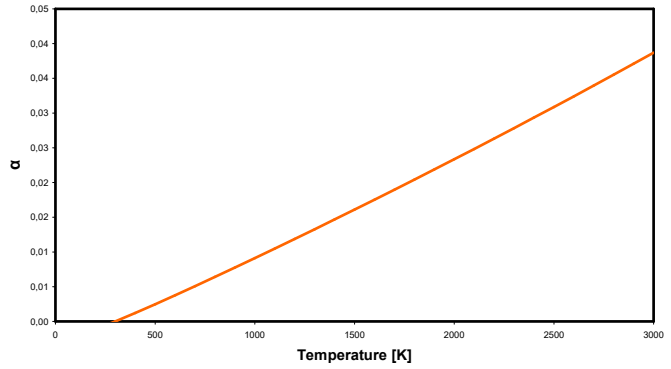

FIG. 3. Coefficient of linear thermal expansion of FeCrAl calculated with BFS.
$\alpha = 8\times10^{-10}\ T^2 + 10^{-5}\ T - 0.0032$, *T in K.*

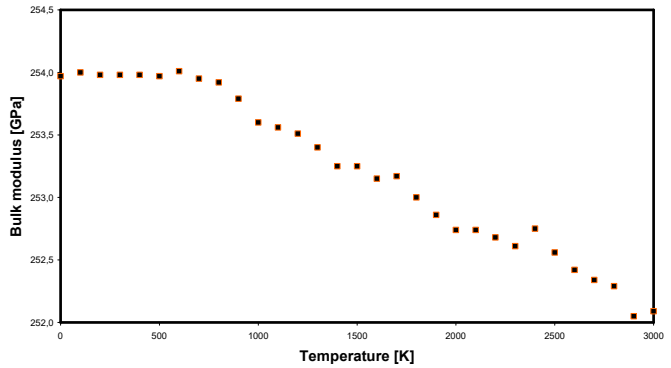

FIG.4. Bulk modulus of FeCrAl calculated with BFS.
$B = 0.1\ T^3 - 5\times10^{-7}\ T^2 + 9\times10^{-5}\ T + 254.02$, *T in K.*

6. METHODOLOGY TO OBTAIN SAMPLES OF FeCrAL

The objective is to obtain a FeCrAl alloy with similar characteristics as those sought for claddings in order to acquire experience and validate calculations. The corrosion resistance of these materials is related to their Cr and Al content. The chemical composition adopted was Fe-13 Cr-4.5 Al (wt. %). The process chart proposed by the research group at Oak Ridge [29] was used as a reference in the present study. It was developed for providing a guide for casting and selecting the appropriate thermo-mechanical treatments for the production of FeCrAl alloys without further alloying aggregates. They were melted starting from pure elements (Fe, Cr, Al) in an electric-arc furnace under Argon atmosphere. After rolling the samples and the preparation of the specimens we proceeds with stress-strain tests at room and 300°C, scanning electron micrographs of the fracture surfaces, dilatometry and chemical analyses.

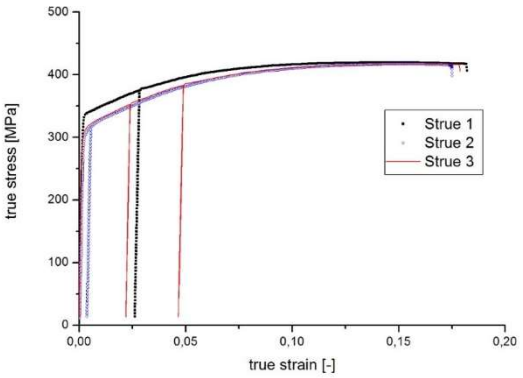

FIG. 5. True stress vs. true strain curves for the three specimens taken from Button #1.

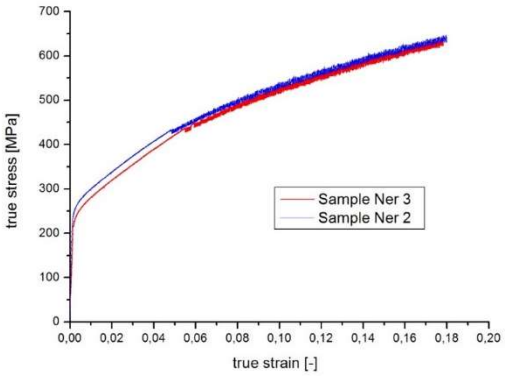

FIG. 6. True stress vs. true strain curves at 300°C for two specimens taken from Button #1.

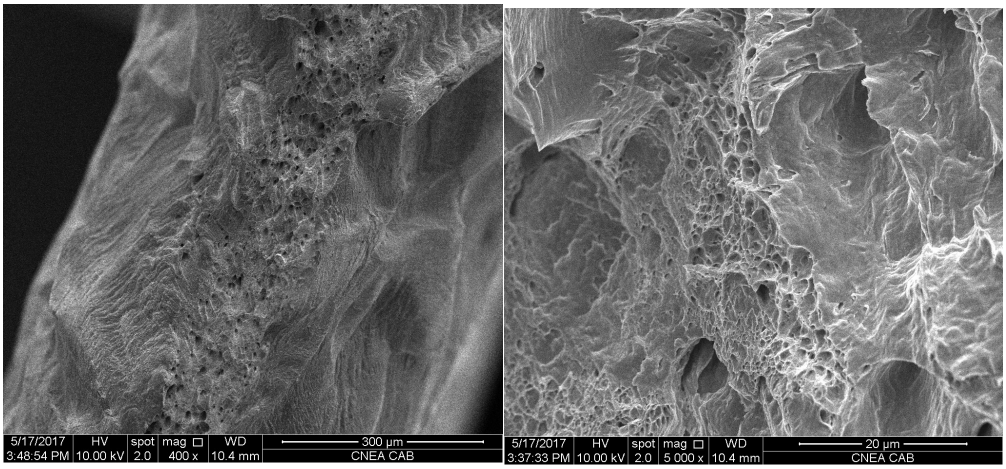

FIG. 7. Fracture surface of Specimen #1 with 400 and 5000 zoom.

Young modulus and UTS were acceptable in comparison with the commercial alloys (see Figures 5, 6, 7 and 8). The fracture surfaces exhibit the typical features of a ductile fracture, after 5% strain in both samples (see Figures 7 and 8), the presence of DSA (Dynamic Strain Aging regime) [46]. The measured thermal expansion coefficient is $\alpha = (11.9 \pm 0.5) \times 10^{-6}$ 1/K (see Figure 9). The result of the chemical analysis was: Fe: 83.25 wt.%, Cr: 13.56 wt.% and Al: 4.30 wt.%. The experimental values obtained will be useful to refine the calculations and to validate the *ab initio* results.

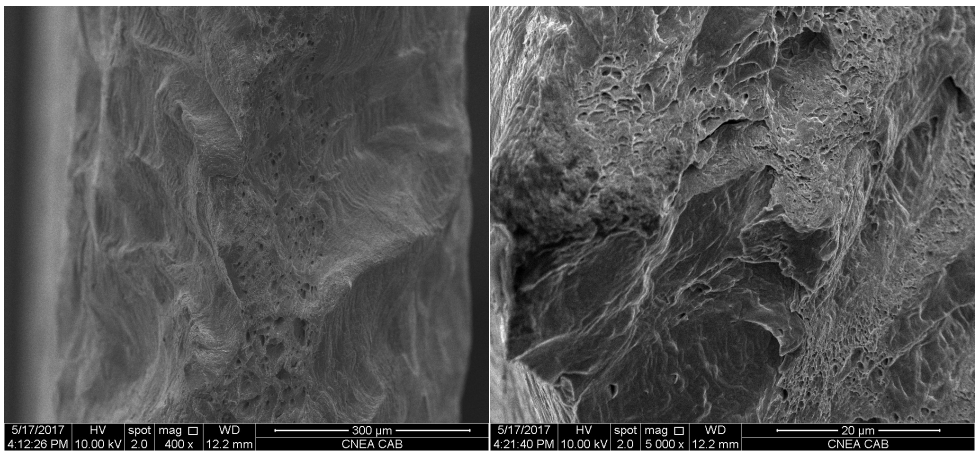

FIG. 8. Fracture surface of Specimen #3 with 400 and 5000 zoom.

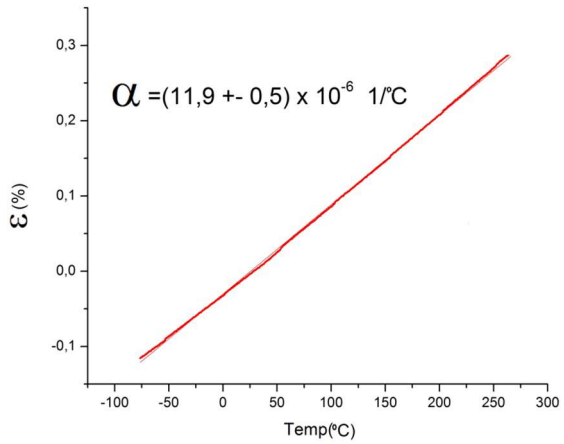

FIG. 9. Dilatometry of our FeCrAl alloy.

7. M³ AND MATERIAL PROPERTIES FOR THE BACO CODE

M³ provides BaCo with the required material parameters and theoretical support the experiments (see for example Figures 10 and 11). The parameters and their dependency with temperature are included in the BaCo code in order to get a preliminary assessment of the expected behaviour of nuclear fuel rods with ATF materials. The Figures 10 and 11 show the calculated values for SiC with QE and experimental measurements for the coefficient of linear expansion and the Young Modulus. The Figure 10 shows the BFS calculation for FeCrAl of the coefficient of linear expansion and the comparison with experimental values and our measurements for our first FeCrAl alloy under development in CAB-CNEA [30, 31]. Excellent agreements were found for those materials in particular in the temperature range of operation of the nuclear fuel.

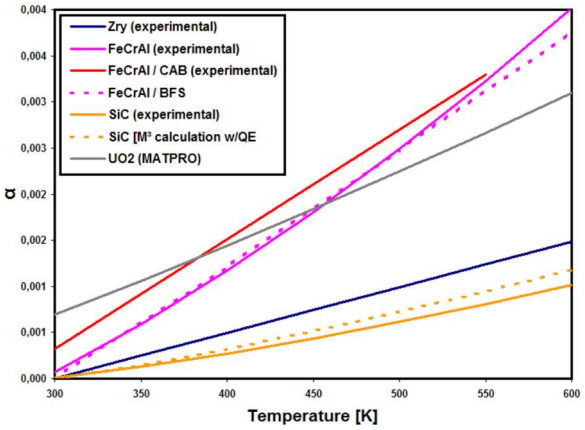

FIG. 10. Coefficient of thermal expansion as a function of temperature for materials currently under study for ATF including our calculation with BFS for FeCrAl and Quantum Espresso ("QA") for SiC).

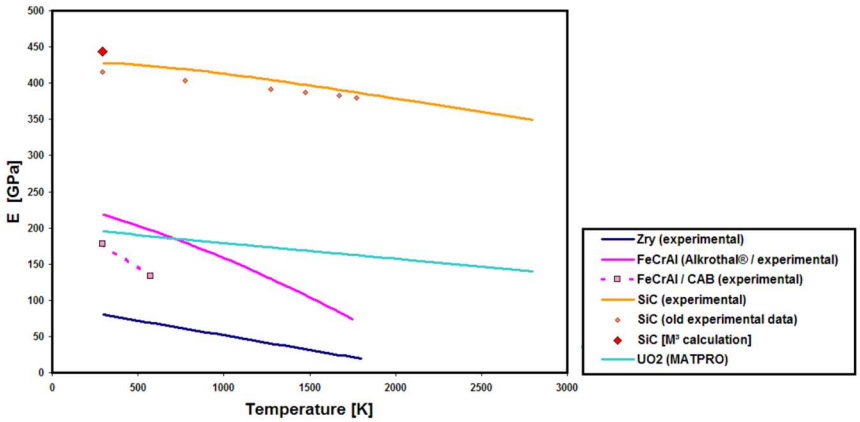

FIG. 11. Young's module as a function of temperature including our calculation by M³.

The calculations are included in the BaCo code. The use of these theoretical correlations is emphasized due to the closure of the HRP and the lack of other irradiation facilities sufficient to cover the current needs of studies under irradiation conditions for ATF and Gen-IV initiatives. M³ synergistically provides a deep support for the development of nuclear materials as shown in the case of claddings using SiC or FeCrAl. The simple calculations suggest a good agreement with the current data.

8. THE BaCo CODE

BaCo is a code for simulating a cylindrical fuel rod's thermo-mechanical and fission gas behaviour under operating and storage conditions. The mechanical and thermal treatment descriptions as well as the pellet, cladding and constitutive equations are available in Ref. [32] and an expanded code definition is included in Ref. [33]. BaCo's modular construction is compatible with various material properties for all fuel rod components (such as SiC and FeCrAl for cladding and USi and UN for fuel as well as data is available). BaCo3D tools [34], full core calculations [35], statistical analysis [36] and post-processing visual information improve application quality and calculation analysis [33]. For each fuel design, new materials imply a whole new set of parameters and models. M³ ("Multiscale Modelling of Materials") is intended to provide analysis of these properties. We highlighted the function of the CRPs organized for the IAEA as D-COM [37], FUMEX, FUMEX I, FUMEX II [38–40], FUMAC and ACTOF in fostering international cooperation in the field of modelling nuclear fuel and establishing codes of fuel behaviour.

8.1. An ATF with alternate claddings (SiC, FeCrAl)

Ref. [41] provides an evaluation of the behaviour of an ATF by using the BaCo code under operating, demanding and storage conditions where it was used some properties of SiC and FeCrAl calculated by the ab initio methods described in previous sections. The simulations were performed with a version of BaCo by using cladding material parameters from the open literature and some properties of SiC and FeCrAl calculated by the ab initio methods described in the previous sections. The Figures 8 and 11 of Ref. [41] shows PCI at the end of the irradiation. That is not a permissive condition and it could initiate a failure in the cladding. Instead, a cladding type SiC/SiC (inner solid pipe filled with fibres) could avoid this failure.

8.2. BaCo3D simulations

Some of the various proposed new materials in the ATF literature are UN, UC, U_3Si_2, ThO_2 and ThC. Figure 12 describes the BaCo simulations of the radial pellet deformation profile for each material using equivalent irradiation conditions. The decrease/increase in ridges and radial displacements of the form of each pellet is clearly seen. Figure 13 depicts the deformations of a solid pellet with a central hole like those of the WWER [42]. It can be seen that the hole's existence increases stress release and decreases PCI.

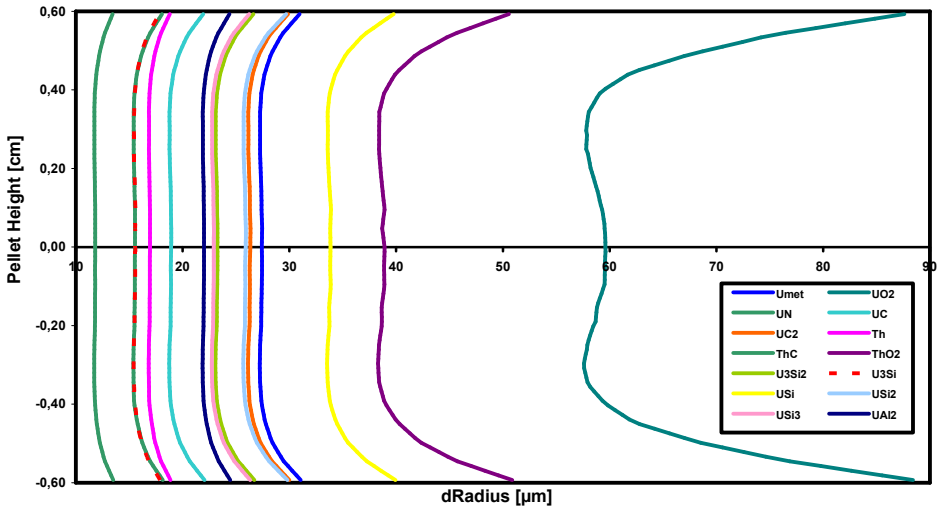

FIG. 12. Radial deformations of several pellets with different nuclear fuel materials irradiated in equivalent conditions.

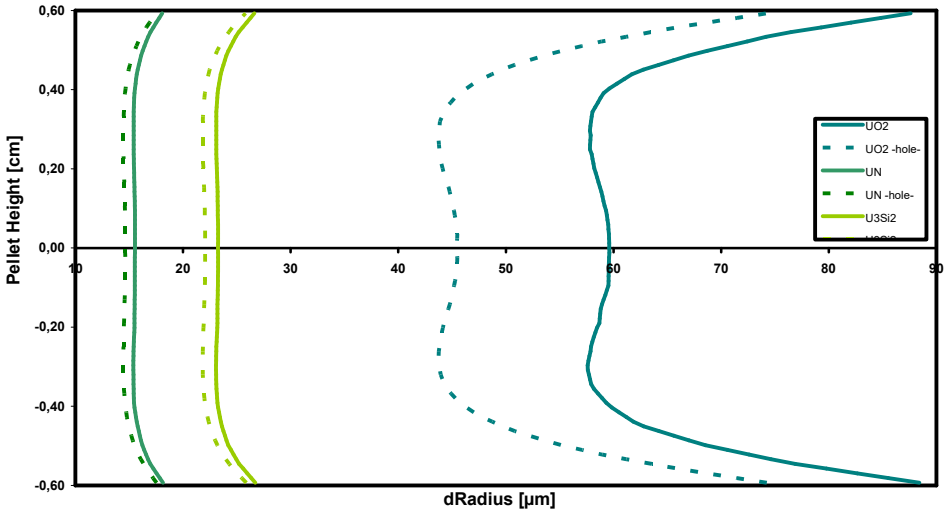

FIG. 13. Radial deformations of several pellets with different nuclear fuel materials irradiated in equivalent conditions with and without a central manufacturing hole.

9. IAEA CRP ACTOF'S SECOND BLIND TEST CASE

9.1. Proposal

The second proposal for a blind test comparison was prepared for Dr. G. Pastore [43]. The data used for the calculations are included in Ref. [43]. These second round of calculations were made in order to fix bugs, to improve the modelling, to assess the simulations and as a base for code comparison.

The approach used for the fast flux is the linear heat rate multiplied by 3×10^{13} (n/m^{2}s)/(W/m). For a LHR of 25 kW/m, this yields a fast flux of 7.5×10^{17} n/m^{2}s, or 7.5×10^{13} n/cm^{2}s.

Requirements of calculation for code comparison:

— Hoop strain at cladding inner and outer surfaces (see Figure 14 and 15);
— Hoop stress at cladding inner and outer surfaces (see Figure 16 and 17);
— Fuel-cladding radial gap width (see Figure 18);
— Oxide layer thickness (see Figure 22);
— Fuel centreline temperature (see Figure 19);
— Rod inner pressure (see Figure 20);
— Fission gas release (see Figure 21).

9.2. Results with BaCo

The BaCo code results are includes in a graphical environment in order to be compared with the other participants of the CRP. It was required only the calculations of FeCrAl and Zry claddings but with we are including our results for a solid SiC cladding. Figures 14 to 22 shows the curves required for the code comparison. The power history includes a shutdown at EOL ("End of Life") and finally room temperature conditions.

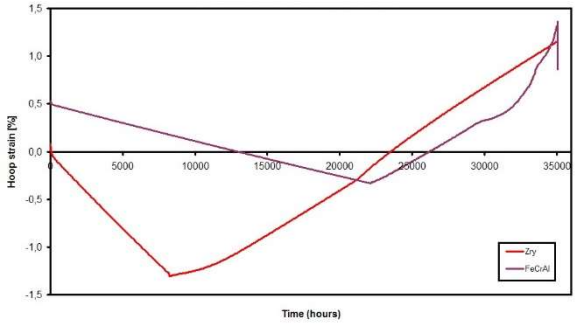

FIG. 14. BaCo calculation of the hoop strain at the inner cladding surface.

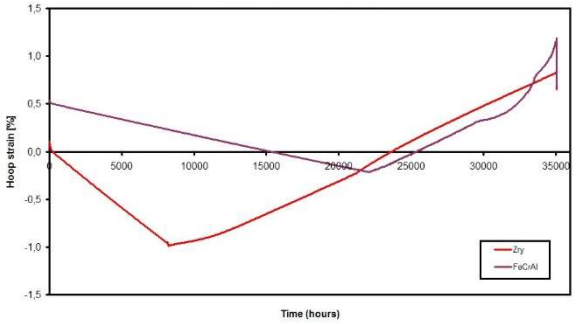

FIG. 15. BaCo calculation of the hoop strain at the outer cladding surface.

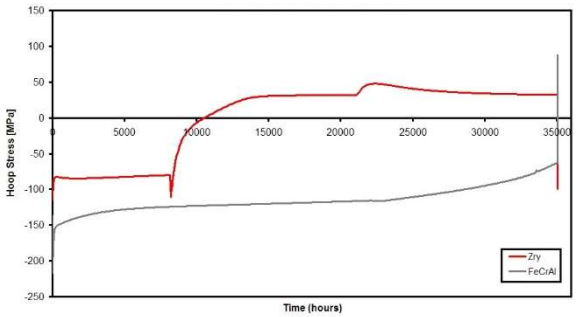

FIG.16. BaCo calculation of the hoop stress at the inner cladding surface.

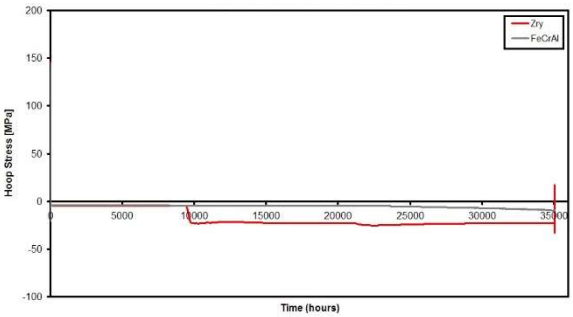

FIG. 17. BaCo calculation of the hoop stress at the outer cladding surface.

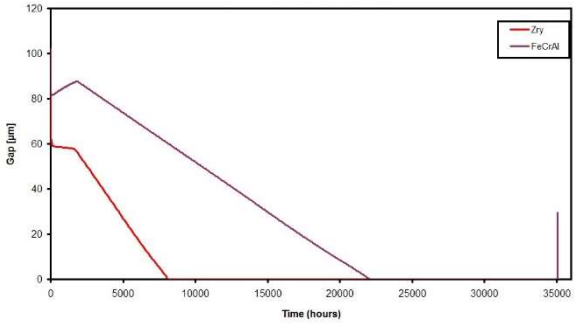

FIG. 18. BaCo calculation of the fuel-cladding gap width.

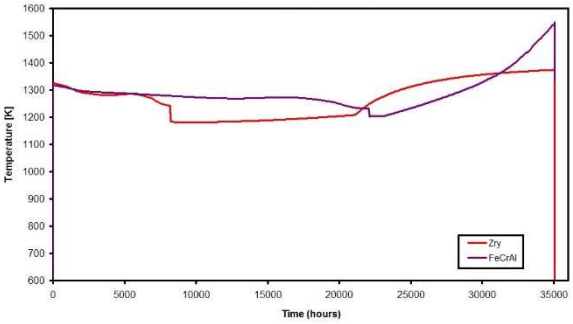

FIG. 19. BaCo calculation of the pellet centre temperature.

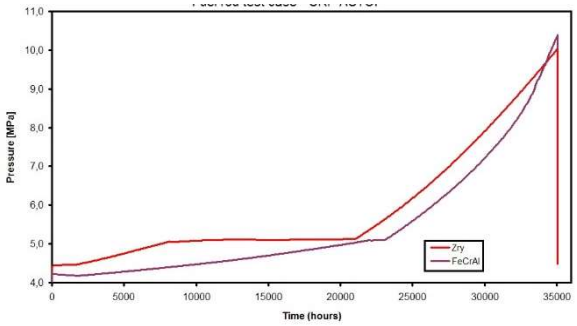

FIG. 20. BaCo calculation of the fuel rod inner gas pressure.

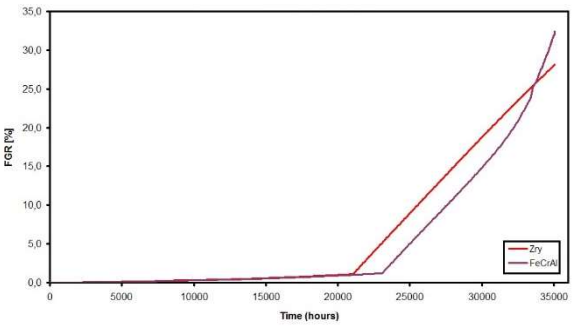

FIG.21. BaCo calculation of the fission gas release.

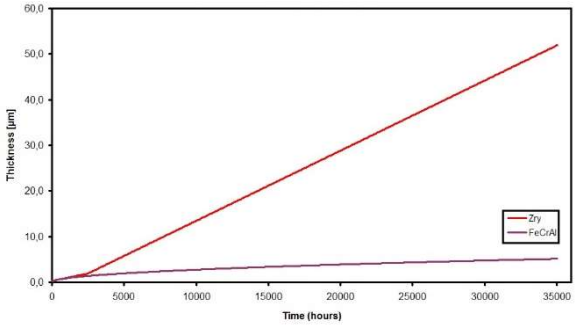

FIG. 22. Cladding oxide thickness.

9.3. Complementary plots

The following plots are included in order to clarify previous results:

— Pellet radius (see Figure 23);
— Gap, pellet and Zry inner cladding radius (see Figure 24);
— Gap, pellet and FeCrAl inner cladding radius (see Figure 25).

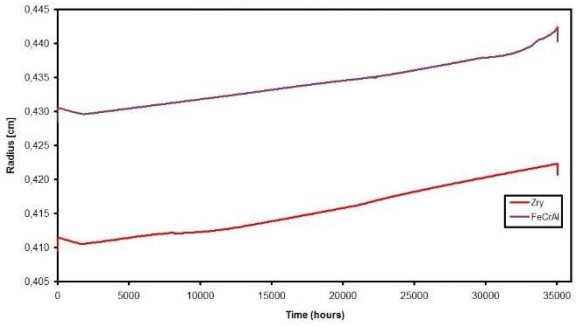

FIG. 23. Fuel pellet radius.

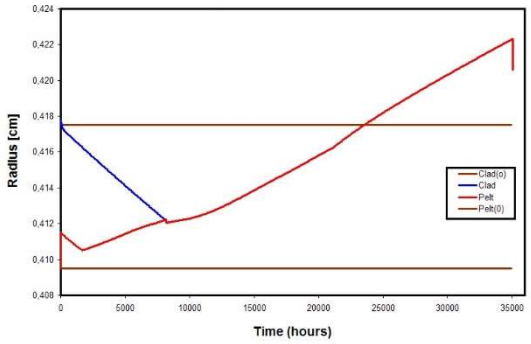

FIG. 24. Evolution of the gap, pellet and inner Zry cladding radius using the as fabricated radius as reference.

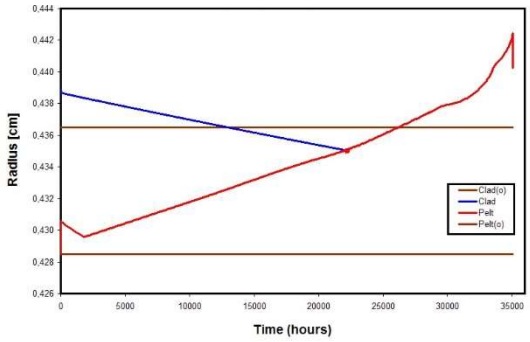

FIG. 25. Evolution of the gap, pellet and inner FeCrAl cladding radius using the as fabricated radius as reference.

The present calculations made with BaCo are different of the previous presented at the 2nd RCM of the CRP ACTOF due to the enhancement of the models of SiC and FeCrAl. These ones are following the recommendations of the CRP ACTOF and our M³ modelling. The curves of the previous plots are satisfactory. Models and programming needs a more complete evaluation and discussions with the participant of the blind test. Weak points: creep of the FeCrAl and cladding thickness oxide of Zry.

10. A NEUTRONIC APPROACH TO AN ATF PROPOSAL FOR PHWR

10.1. Neutronic calculation of an ATF with a FeCrAl cladding

In order to understand and implement new cycle length and reactivity mitigation techniques based on the neutron balance in the systems, the development or enhancement of new materials for Accident Tolerant Fuels involves studying its neutronic behaviour.

The design of the new materials for PWR and PHWR technologies will be evaluated. But for a CANDU reactor, only the full cost effect analysis in the Nuclear Fuel Cycle will be performed. The present study will therefore concentrate on CANDU fuel elements as Argentina has the license to produce and develop this technology. As a result, the availability of accurate data for this study will be a benefit; the neutronic measurement code to be used is DRAGON Code [44]. WIMS D4 was the library used to calculate burnup. A library containing 64 energy groups and 167 isotopes, given by the code (and established by IAEA).

The cladding materials studied were FeCrAl [29] and SiC [45], both alternatives being proposed to replace the current clad of Zry (zircaloy) currently used in the nuclear industry.

10.2. FeCrAl as cladding from neutronic point of view

The advantages of the FeCrAl are associated with the enormous experience in the steel industry, since it belongs to this family. But it has to be accounted that being part of the steels family it increases the absorptions of the system with a consequent need of increase of the enrichment above allowed levels to maintain the reactivity.

10.3. SiC as cladding material from a neutronic point of view

SiC is a ceramic with all that implies. First it does not modify the absorptions of the system. But, as a ceramic material it has issues to be solved from the behavioural point of view of the fuel element since it is fragile and cannot stand PCMI ("Pellet Cladding Mechanical Interaction").

10.4. Description of the work

A unit cell and cluster calculations were performed to show the evolution and the dynamic of the reactivity in PWR (first) and CANDU fuel rods (in second place). Different enrichments were taken into account to compensate the reactivity loose due to the increase of absorptions in some cases and as a consequence, an extension of the fuel cycle was reached. These results will combined with the economic calculations, where the length of the cycle will depend strictly on the residence time of the fuel element in the reactor.

10.5. PWR fuel rod calculations

10.5.1. Calculation of Reactivity at a Unit Cell as a Function of Burnup for normal clad and FeCrAl alloy with UO_2

In three different cases, a cell analysis was performed with a simple discretization in order to evaluate the reactivity change due to a particular cladding product like FeCrAl. First, it was calculated k_{inf} for a 4.2% enrichment UO_2 and Zry-4 clad, then, for a FeCrAl clad with the same concentration of ^{235}U and finally for the same FeCrAl fuel rod, but with 50% less thickness in the clad. The same thickness for the case of Zry-4 and FeCrAl alloy has much higher neutron absorption for FeCrAl. On the other direction, it should be taken into account that a steel's mechanical strength is generally much higher than the base alloys of zirconium, which is why a reduction of the cladding thickness to tolerable manufacturing values was suggested and how much absorptions decreased was examined in this way (see Figure 26).

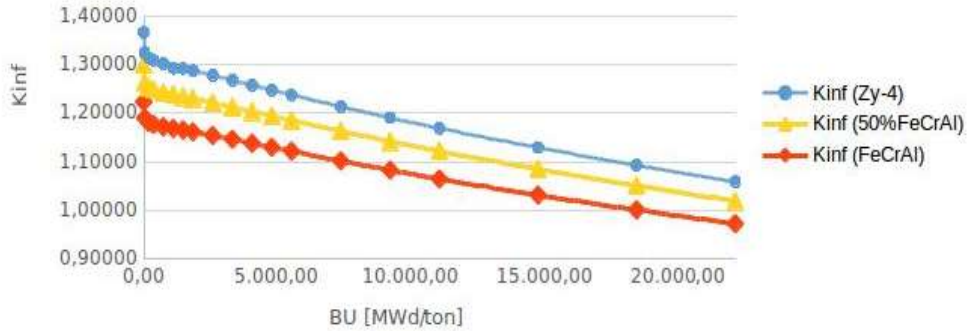

FIG. 26: k_{inf} evolution for the unit cell vs burnup for different cladding materials and thickness.

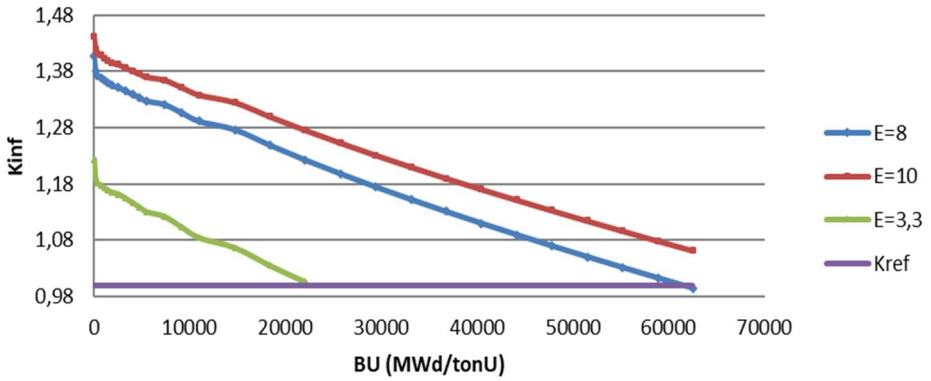

FIG. 27. Reactivity values for the same fuel rod with different enrichments.

It is possible to see that even reducing the thickness of the cladding in a half, it is not possible to reach the original values of k_{inf} (and its consequent cycle length), fact that is base design for these new fuels. Therefore, the value of the enrichment necessary to obtain values of k_{inf} similar to those with a Zry clad and a standard thickness was evaluated.

It can be seen from Figure 27 that the enrichment necessary to be able to have a k_{inf} able to sustain a reaction during a complete cycle or more with a fuel rod with FeCrAl is about 8%. This value exceeds the proliferation limits currently used, so it would not be feasible to put it into practice. On the other hand, an optimum between enrichment and thickness should be analysed, and a core analysis should be performed to evaluate these effects together with reactor leakage, although this would not improve current results.

Another drawback of this analysis is that the extension of the cycle to more than 60 MWd/kgU should be accomplish with an analysis of the length of the batch to match them in order not to modify the original strategies of maintains off the grid. If we taking into account that these strategies are planned considering seasonal issues and are pre-defined by the utility should not be modified by an improvement on the fuel element (see Figure 28).

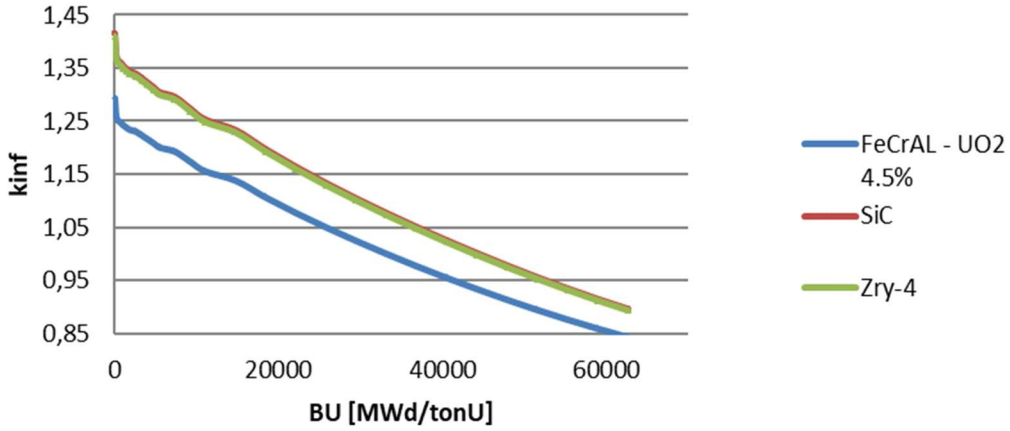

FIG. 28. Reactivity evolution for the three different claddings in study with 4.5% ^{235}U content.

10.5.2. Calculation of Reactivity at a Unit Cell as a Function of Burnup for normal clad and SiC alloy with UO_2

There is no considerable change in reactivity with SiC compared with the base case of Zry-4. Considering this issue, SiC is proposed as a very interesting material from the point of view of neutronics and the reactivity loose in the reactor but taking into account the fabrications drawbacks and the lack of sufficient knowledge about its behaviour during operation PCMI it would not be one of Argentina's choice for the short term development.

10.6. Improvements on PHWR reactors

10.6.1. FeCrAl on CANDU Reactors

From the perspective of Argentina, it is important to evaluate these new materials in its reactor types. Argentina has three PHWR type rectors, two of them are Siemens design and one is a CANDU design. In that way a comparative analysis of the results with different enrichments were done to a typical CANDU FE in a pressure tube as part of the first analysis taking into account that Embalse (the CANDU type reactor), is on rebumping stage. So any improvement on the fuel element should be done at this stage for the next operational period.

For a first approximation to a PHWR fuel assembly, we have performed a simulation of a CANDU fuel element in a pressure tube replacing the cladding by a FeCrAl alloy. In Figures 29 and 30 is shown the multiplication factor plot for U_{nat} with Zry-4 combination of the original design and the comparison with the replacement of the original cladding with FeCrAl alloy.

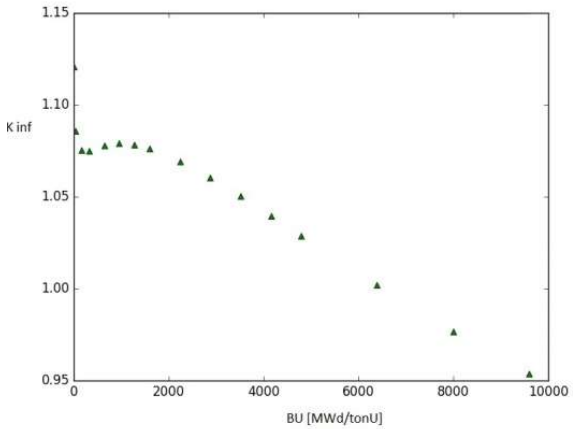

FIG. 29. Original CANDU Cell K_{inf}.

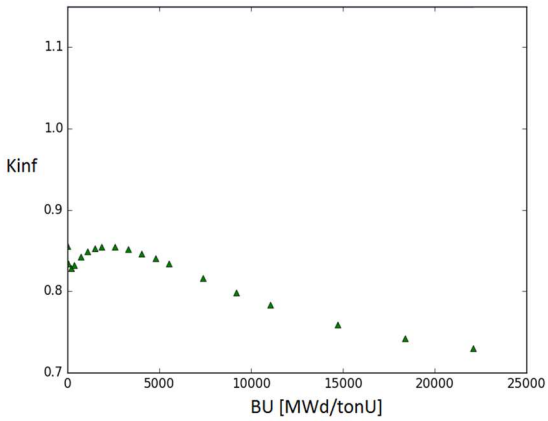

FIG. 30. K_{inf} for a CANDU FE with FeCrAl alloy as cladding and natural uranium.

It can be seen that with the only introduction of the improvements on the cladding, the reactivity of the FE will not be enough to maintain the reaction. In order to overcome the increase of absorptions in the system we decided to perform a sensitivity analysis to estimate the minimum enrichment to supplement the loose of reactivity.

From Figure 31, it can be seen that the minimum enrichment to obtain, at least, the same burnup as a CANDU FE is 1.3%. From the point of view of an extension of the cycle, with 3.3% enrichment, the cycle could be extended to almost 17000 MWd/tU. Taking into account the average power density, this burnup reflects an increase of 500 days of the FE in the reactor (Figure 32).

The possibility of varying the thickness of the cladding was considered and the extension of the cycle was calculated for the different cases. In the first place, it was proposed to use the "optimal" enrichment from the situation of original thickness and extraction burnup equal to the original cycle (enr = 1.3%). In this way, it was the gain in days of the cycle and its respective economic savings.

The results obtained for this proposal, that is, with fixed enrichment in 1.3% and varying the thickness can be seen in Fig. 33.

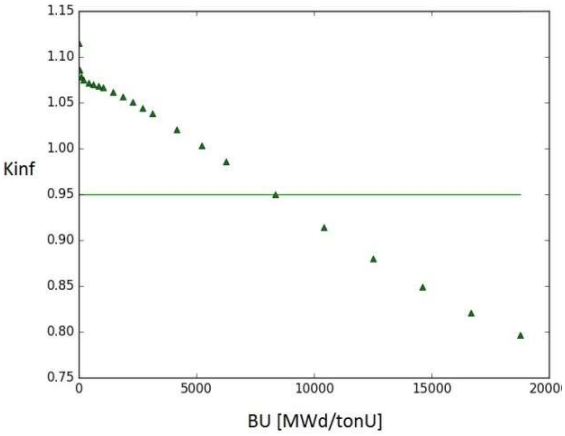

FIG. 31. K_{inf} with an enrichment of 1.3% with FeCrAl clad.

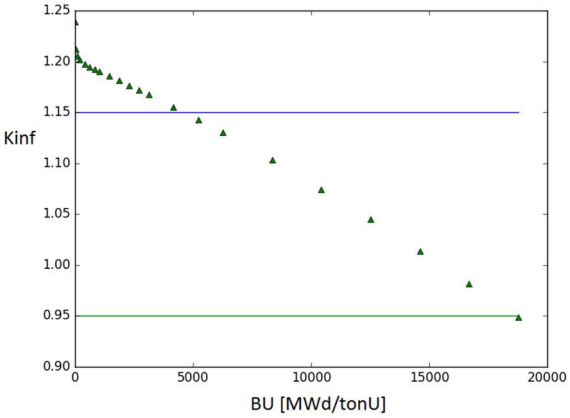

FIG. 32. K_{inf} with an enrichment of 3.3% FeCrAl clad.

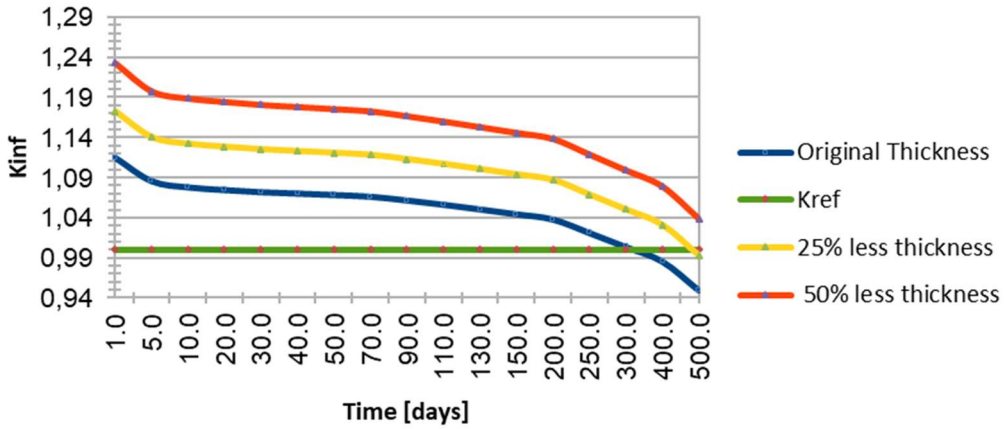

FIG. 33. Evolution of the multiplication factor for different thickness of FeCrAl cladding.

As expected, for the smallest thickness of the clad, the longest duration of the cycle was found with almost 600 days of irradiation. This is to be expected by two effects that are added as the decrease of the absorptions in the material of the cladding and the increase of the fissile material as compensation of the space generated in the fuel. But this decrease of the thickness is not feasible considering the original thickness of a CANDU fuel element. In order to compare the results of the different enrichments analysed for the FeCrAl alloy with a commercial 316 Stainless Steel, the same procedure was performed and similar results were found as Figure 34 shows.

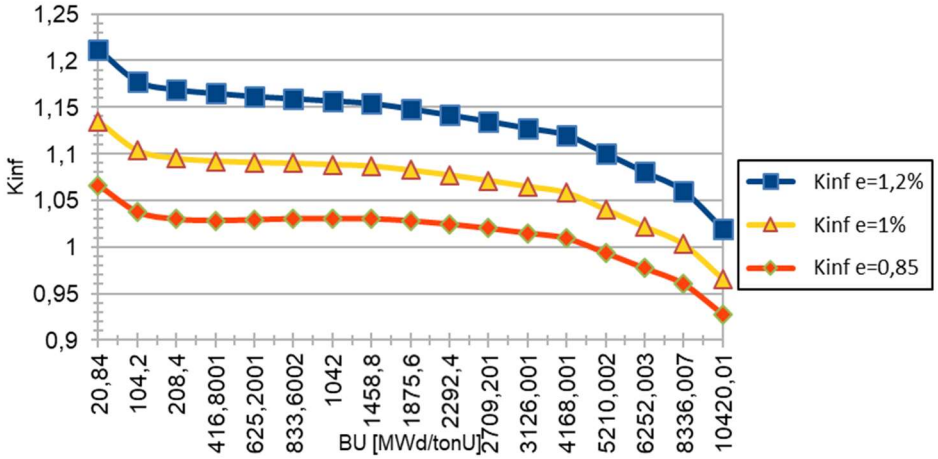

FIG. 34. Evolution of the multiplication factor for different enrichments with Stainless Steel as cladding.

10.6.2. SiC on CANDU reactors

As was expected there is no major change on reactivity, actually, there is a small increase in reactivity due to lower absorptions in the system (see Figure 35).

A CANDU fuel is not compatible with the use of a SiC cladding. The advantage of the good neutronic behaviour is not enough to validate a SiC cladding for a CANDU fuel. A CANDU cladding is a collapsible one. Pellet and cladding of the fuel rod are in contact during the entire irradiation as it was defined by the CANDU designers. The thickness of the Zry-4 cladding of the CANDU is the smallest one used in the entire nuclear fuel designs. The CANDU fuel rod is designed in order to works under compression stresses. Nevertheless, during operation, we find stress reversal and PCI-SCC. That behaviour is not acceptable for a solid SiC cladding or for a modern SiC cladding with three layers (solid/fibbers/solid).

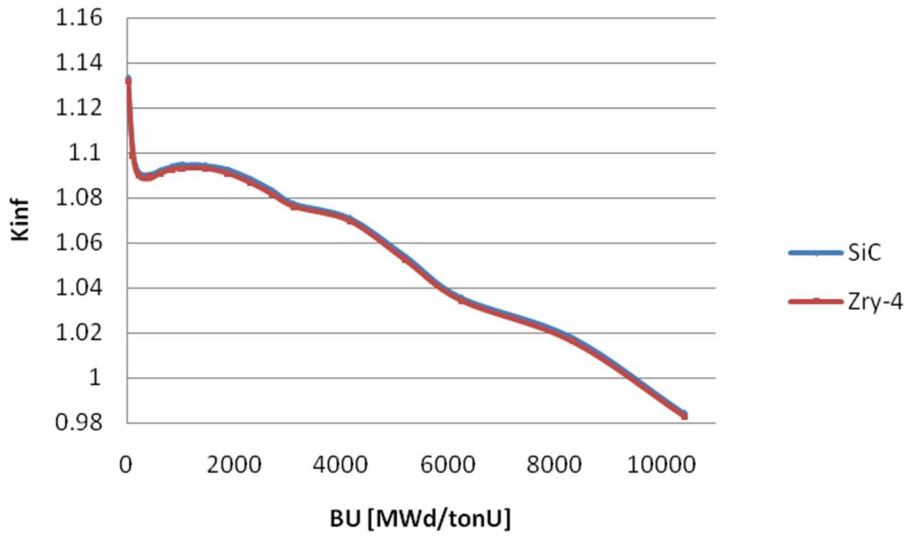

FIG. 35. Comparison of the multiplication factor for SiC and Zry-4 claddings.

10.7. Further developments regarding neutronic implications on ATF's cladding materials

This first calculation stays the first step on the neutronic behaviour of these materials in PWR and CANDU systems.

It is important to stand that further calculations regarding reactivity coefficients and core calculations need to be done.

One of the main remaining questions is if the power reactivity coefficient in CANDU can change its sign.

10.8. Economic implications of FeCrAl on CANDU FE

From an economic point of view, these changes imply an increase in the FE's costs, but as a result of a balance of the benefits and its cons, if more energy is delivered, a longer amortization term can be used depending on the life of the FE in the reactor core.

10.8.1. Description of the work

For the present analysis a study from the grave to crave was performed in two situations. First we presented the case of natural uranium for a typical CANDU fuel element to evaluate the Argentinean cost per kg of assembly. Then we present a comparison of the fuel cost with a FeCrAl alloy and the minimum enrichment calculated before to obtain the same cycle length. In Table 1 is show the costs that Argentina has now a days to face during the life cycle of the uranium. The prices only take into account until the dry storage because no decision was taken of what to do with the wastes yet. Taking into account these prices, the losses during the different process and the lead or lag times involved, the final price per kilogram of the fuel element for the whole cycle is 198.45 USD/kgU.

TABLE 1. COSTS OF THE DIFFERENT STEPS OF THE FUEL CYCLE FOR TYPICAL CANDU ZRY-4 – U_{nat}

Unit cost						
Monetary units per lb U_3O_8	Conversion to UO_2 (wet way) Monetary units per kg(U)	Conversion to UF_6 Monetary units per kg(U)	Enrichment price per SWU	Fabrication Monetary units per kg(U)	Transport Monetary units per kg(U)	Dry Storage Monetary Units per kg(U) per year
25	40	7	45	130	5	20

10.8.2. Estimation of the cost of the FeCrAl Alloy in a CANDU Fuel Cycle

Between both cycles there are some differences. First of all, there exists an extra step to enrich the uranium to some level depending on the requirements of the cycle. In this case, we are going to calculate the value to 1.3% to understand the cost structure in order to maintain the same average residence time in the reactor.

Second, the conversion method to UF_6 before enrichment is via dry way is a complete different process with different cost as can be seen in Table 1.

As a consequence of changing the cladding material for the fuel element, the fabrication process will be different and in the next section we are going to analyse deeper the structure of the costs.

10.8.3. Brief analysis of the costs for the fabrication process.

The fabrication process costs could be divided into three different components.

- The cost of the pellets (fabrication, sintering, pressing);
- The cost of the cladding materials;
- The cost of manufacture (workers' salaries, time of machines used, etc.).

The distribution of the costs is 20%, 50% and 30% respectively. The fuel pellets won't change the cost taking into account that the fabrication process won't change. But the materials and fabrication process will change its costs. Table 2 show the unit prices of the Zry-4 and FeCrAl that are available commercially at a reasonable market prizes found about 2018.

TABLE 2. COMMERCIAL PRICE OF ZRY-4 AND FeCrAl TUBES

Zry-4 [USD/tube]	FeCrAl [USD/tube]
100	45

These prices led to a relation of 2.2 to 1 as relative prices. Using this relation and the information that a CANDU FE cost 65 USD/kg of materials we extrapolate linearly the cost of materials and manufacture of a FeCrAl FE for CANDU. The final cost is 78.26 USD/kgU. With this value of fabrication cost, the average cost of the fuel cycle per kgU was calculated in 200 USD/kgU. This value is little over the Zry-4 cladding. This value is estimated, considering that there is no accurate value of the production of the FeCrAl of nuclear grade at industry scale.

10.9. Some remarks about a CANDU ATF factibility

It is possible for a CANDU reactor in a first longer LEU cycle with the benefits of making it more efficient and then begins thinking about changing its cladding material to fully change its fuel cycle by implementing the enrichment technology but with new safety requirements.

Furthermore, needs to be done to understand the neutronic of an enriched CANDU from the safety point of view, taking into account the size of the core. All the reactivity coefficients must be improved but all the calculations need to be done with a core model.

A CANDU fuel element is feasible with enrichment between 1 and 1.3%.

The average cost per kilogram of a CANDU cycle with FeCrAl is very close to the original cost and if the cycle is extended to longer periods with a more resistant cladding, the incomes of the utility must increase leading to a more profitable FE for the technology.

All the economic calculations were done considering a CANDU power plant already installed, so no amortizations cost were taken into account.

We had shown that a SiC cladding is not compatible with the original CANDU fuel design. It is plausible a FeCrAl cladding for a CANDU if we accept the U enrichment. In that case we are losing one of the goals of the CANDU technology: the use of natural Uranium. A more compressive analysis must be done by taking into account the possible changes in the reactor design not only in the fuels.

11. CONCLUSIONS

By taking into account the expected outputs presented during the 2nd RCM of the CRP ACTOF, the following results were arising:

- A new version of the BaCo and BaCo3D codes including cylindrical rods options with new fuel and clad materials used, proposed and/or promising for ATF at least with an illustrative comparison purpose.
  We expect an improvement of the modelling after the 3rd RCM of the CRP ACTOF. The curves of the previous plots are satisfactory. Models and programming need a more complete evaluation;
- Material parameters and correlations for the materials of ATF under an *ab initio* and M³ theoretical support. Thermal conductivity (k), specific heat (C_p), thermal expansion ($\Delta l/l$), elastic constants, density (ρ), Young's modulus (E), Poisson's ratio (ν), net parameters, etc. can be theoretically obtained. The material studies at this stage were SiC and FeCrAl for claddings at they were integrated into the BaCo code. Material parameters of UN, UC, U_3Si_2, ThO_2 and ThC where included in BaCo3D in order to obtain a more realistic 3D stress-strain approach. ThC and *fcc* Th were studied with this approach;
- The BFS method appears as an excellent tool for applications in nuclear materials;
- The BaCo and BaCo3D new features must be most deeply assessed (see below the "*Recommendations*");
- It was concluded the first step of the development of a FeCrAl-based alloy for claddings. The experimental values obtained will be useful to refine the calculations and to validate the ab initio results;
- It is important to further the development taking into account the long experience of the industry with steel-based alloys, moreover considering the good behaviour of this type of claddings;
- The results obtained are close to the values of bibliography, in particular considering the results obtained at room temperature. The results at 300ºC are less consistent considering that the equipment was prepared to handle bigger samples and some adaptation had to be done. In spite of the non-standardized experiments, the results were satisfactory for the first step of the development;
- We can reasonably estimate that a first longer cycle of LEU for a CANDU reactor with the benefits of making it more profitable and then start thinking in changing its cladding material to modify completely its fuel cycle introducing the enrichment technology but with new safety standards. All the reactivity coefficients must be improved but all the calculations need to be done with a core model. A CANDU fuel element could be feasible between 1 and 1.3% enrichment;
- We can reasonably estimate that the average cost per kilogram of a CANDU cycle with FeCrAl is very close to the original cost and if the cycle is extended to longer periods with a more resistant cladding, the incomes of the utility must increase leading to a more profitable FE for the technology;
- The ATF initiative was included in the regular courses of degree of Nuclear Engineering at the Balseiro Institute, Argentina and post degrees courses.

12. RECOMMENDATIONS

- A "MATPRO" for ATF and Gen-IV fuel materials;
- It is emphasized that there are not enough data of irradiations and the HRP was closed;
- Encourage the IAEA to coordinate ASAP a CRP for ATF simulations following the guidelines of the previous CRP FUMEX I, II and III, and the blind test included in CRP ACTOF. This CRP must be focused in the normal and extreme conditions of operation of the ATFs because at present it is an unknown;
- Analyse the plausibility of a CRP about M³ ("Multiscale Modelling of Materials") for ATF and Gen IV materials;
- An "open" IFPE for ATFs.

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