# PRESENT AND FUTURE TRENDS IN PHWR FUEL MATERIAL MODELING WITH THE BACO CODE

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## ABSTRACT

The BaCo code (Barra Combustible, Spanish expression for "fuel rod") was developed to simulate the nuclear fuel rods behavior under irradiation. The generation of nucleo-electricity in Argentina is based on PHWR NPP and, as a consequence, BaCo is focused on PHWR fuels keeping full compatibility with PWR, WWER, among others type of fuels (commercial, experimental or prototypes). BaCo includes additional extensions for 3D calculations, statistical improvements, fuel design and batch analysis. Research on new fuels and cladding materials properties based on *ab initio* and multiscale modeling are currently under development to be included in BaCo simulations.

## INTRODUCTION

The BaCo code was developed at the end of the 70´s in the Atomic Energy National Commission of Argentina (CNEA) with the purpose of studying the fuel rod behavior under irradiation conditions [1, 2]. Although the first applications of this code were related with the study of the effect of different empirical models on the fuel rod behavior, the BaCo code currently gives the modeling support for the design of advanced PHWR (CARA fuel [3]) and innovative PWR fuels (fuel for the CAREM reactor [4]). The confidence in the results regarding the description of the fuel behavior under irradiation enables the inclusion of the BaCo code in several international fuel code comparison programs as D-COM, CRP FUMEX I and II, and, at present, in the CRP FUMEX III of the IAEA. Although the development of BaCo was focused on PHWR fuels, as CANDU [5] and Atucha ones [6], the code holds a full compatibility with advanced, experimental, prototypes and/or unusual fuels as PWR, BWR, WWER and PHWR MOX. Currently, the BaCo code includes additional tools as the software package for finite elements 3D calculations [7] and the statistical improvements for advanced fuel designs [8]. BACO allows the calculation of a complete set of irradiations as for example the calculation of a full reactor core [6].

It is of crucial importance nowadays to develop a better experimental and theoretical knowledge of the processes related with the evolution of defects and the accumulation of fission products for modeling the fuel behavior under different operating conditions and the evolution of a spent fuel over long period of time. The current experimental database could be enough to support empirical correlations and modeling 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. The unavailable data needed for new fuels development will be obtained through a multiscale modeling, a methodology that will provide the theoretical approach to model the properties of materials through *ab initio*, molecular dynamics, kinetic Monte Carlo and finite elements calculations over the relevant length and time scales of each method [9].

In this paper we present the main BaCo code features in the area of PHWR nuclear fuel design, an overview of the BaCo code results of the PHWR cases included in the CRP of the IAEA and the comparison of experimental CANDU fuel of India in order to illustrate the difficulties to obtain a strong experimental support for the models [10]. It is also presented an overview of the use of BaCo with new fuel materials, a new field of application as the fuel storage and the preliminary developments in fuel materials through a multiscale modeling.

## THE BACO CODE

### Main Issues of the Code

The BaCo code was developed at CNEA for simulating nuclear fuel rods behavior under irradiation [1]. The development of BaCo is focused on PHWR fuels behavior under irradiation, as CANDU and Atucha ones, and during storage conditions but, it keeps a full compatibility with advanced fuels, as for example uranium nitride and carbide.

BaCo assumes azimuthal bi-dimensional symmetry in cylindrical coordinates for the fuel rod. Although angular coordinates are not considered explicitly, angular dependent phenomenon, as well as radial cracking, are simulated through the angular averaging method [2]. The hypotheses of axial symmetry and modified plane strains (constant axial strain) are used in the numerical modeling. The fuel rod is separated in axial sections in order to simulate its axial power profile dependence. The BaCo code structure, models, constitutive equations, mechanical and thermal treatment have already been described in reference [1]. The strategy for the development of the code is presented in reference [2] with a brief description of the code.

The modular structure of the code easily allows the description of phenomena such as elastic deformation, thermal expansion, creep, swelling, densification, restructuring, cracks and fission gas release, observed in the $UO_2$ pellet behavior. For Zircaloy (Zry) cladding, the code is able to model the elastic deformation, the thermal expansion, the anisotropic plastic deformation, and creep and growth under irradiation.

The current version of BaCo can be applied to any geometrical dimensions of cylindrical fuel rods with $UO_2$ pellets (either compact or hollow, with or without dishing) and Zry cladding. It is important to note that the special features of the BACO code allow a complete treatment of the fuel with or without mechanical contact between the pellet surface and the clad at any irradiation stage. It could be fully used to model self standing clad sheets (like LWR and Atucha fuel rods) or collapsible clad sheets (like CANDU and Embalse fuel rods) [5] with no special changes in the physical models triggered by the user input.

Fuel rod power history and cladding or coolant outside temperatures must be given as input to the program. Rod performance is numerically simulated using finite time steps (finite differential scheme). The code automatically selects time steps according to previously defined physical and numerical criteria [1]. The code output includes the distribution of the following variables along the rod axis: temperature profiles for pellet and cladding, main stresses at pellet and cladding, radial and axial crack pattern in the pellet, main strains and hot geometry of pellet and cladding, change in porosity, grain size and restructuring of the pellet, fission gas release to the free volume in the rod, trapped gas distribution in the fuel and in the $UO_2$ grain boundary, internal gas pressure and current composition of the internal gas, dishing shape evolution.

BaCo is currently used for fuel prototypes design, analysis of the expected performance and development of future irradiation tests for the CARA Fuel Project [11] and the CAREM reactor fuel [4].

**Advanced Features of BaCo**

BaCo 3D tools [12], statistical analysis [8], full core calculations [6] and data post-processing improve the code performance and the analysis of the results. Although the BaCo code uses a quasi-two-dimensional approach, the use of several three dimensional (3D) finite element features allow a complementary analysis of 3D properties, as for example the stress-strain state at a specific period of time during the irradiation. The BaCo code results were enhanced by using “ad hoc” tools developed at the MECOM and DAEE Divisions (Bariloche Atomic Center, CNEA). The temperature profile, the crack pattern and the boundary conditions (as the inner pressure, pellet stack weight, etc.), among others, are calculated with BaCo as the input data to MECOM tools. The 3D stress-strain state and the deformations of the $UO_2$ pellet [12] are calculated subsequently.

For a better understanding of the uncertainties and their consequences, the mechanistic approach must therefore be enhanced by the statistical analysis. BaCo includes a probability analysis within their code structure covering uncertainties in fuel rod parameters, code parameters and fuel models. As consequence, the influence of some typical fabrication parameters on the fuel cycles performance can be analyzed. It can also be applied in safety analyses and economics evaluation to define the operation conditions and to assess further developments [8]. These tools are particularly valuable for the design of nuclear fuel elements since BaCo allows the calculation of a complete set of irradiations. As an example, BaCo was used to calculate the fuel behavior indicators, like stresses, temperatures, dimensions, pressures and gasses releases of all the fuels of the first SEU core of the Atucha I NPP by using the detailed power histories of each fuel [6].

## BACO CODE RESULTS

**The PHWR cases of the CRP FUMEX II**

CNEA was a participating member of the IAEA Coordinated Research Project (CRP) on “Improvements of models used for fuel behavior simulation (FUMEX II)” [13] with the BaCo code. This initiative was an international effort to enhance the knowledge on nuclear fuel behavior.

The CANDU fuels are characterized by: short length (about 0.5 m), thin cladding, no plenum, natural $UO_2$, normal pressure of the filling gas, horizontal position during irradiation, etc. CANDU is an extremely simple fuel (six pieces, four materials and four types of welding). The burnup at EOL of a CANDU fuel is ~7 MWd/kg$UO_2$. The

cladding is collapsible due to the low thickness of the cladding and the lack of over-pressure inside the rod. As for the PWR, the present trends in the CANDU technology includes the increment of the number of fuel rods (decrement of the linear power) and burnup extension (with SEU), as the CANFLEX and CARA fuels [3]. The starting point of a CANDU code is the assumption of a pellet stack with the clad collapsing over the pellets, and as consequence, it looses a full compatibility with PWR fuels. That is not the situation for the BaCo code because it can simulate all situations, i.e., open and closed pellet-cladding gap.

The use of CANDU cases in the CRP FUMEX II was a good challenge for all the participants, not only for the COG ("CANDU Owners Group"). The CRP FUMEX II did not include a real case for CANDU fuel and the two selected cases were simplified ones. Those data were prepared by AECL (Canada) as an exercise of fuel design review and participated in the CRP FUMEX II with the ELESTRES code. Those exercises should be understood as a comparison between the codes of AECL and the rest of the participants, in particular Argentina, Korea, India and Rumania.

***Example 1: Effect of Power on the Fission Gas Release (Case 27 (3a))***

The purpose of this computational experiment was to study the effects of linear rating on fission gas release by comparing the differences between codes via parametric studies. The main aim was to identify regions where models differ significantly. The power histories were a series of constant linear powers in the range 10-60 kW/m up to a burnup of 800 MWh/kgU. It is important to note that the calculated pressure arises over a conservative pressure level if we take into account that the coolant pressure is ~12 MPa (see Figure 1). The same trends and values were calculated for Profess –BARC– (see Figure 2), START-3 –VNIINM–and ELESTRESS –AECL– [9]. The calculations were inconsistent due to overpressure above a linear power of ~400 W/cm. The best ways to enhance the design of this hypothetic Hi-Bu CANDU fuel is to increase the plenum volume. Nevertheless a CANDU fuel has no plenum. A final conclusion should be that an increment of the rod free volume could be done just with the increment of the dishing volume or with a special design of the end caps.

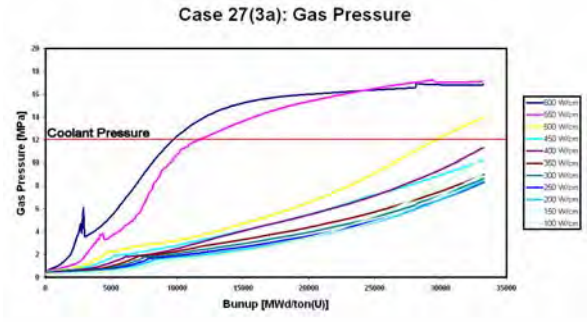


Fig. 1: Internal gas pressure (BaCo, CNEA, Argentina). Coolant pressure as reference.

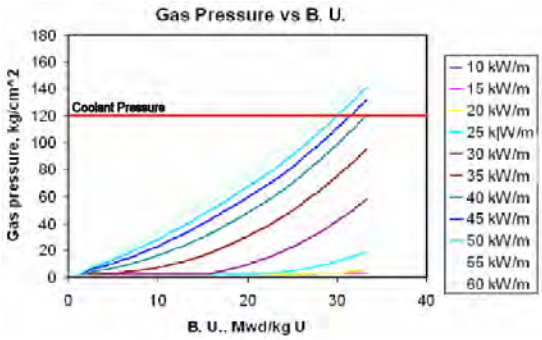


Fig. 2: Internal gas pressure (Profess, BARC, India).

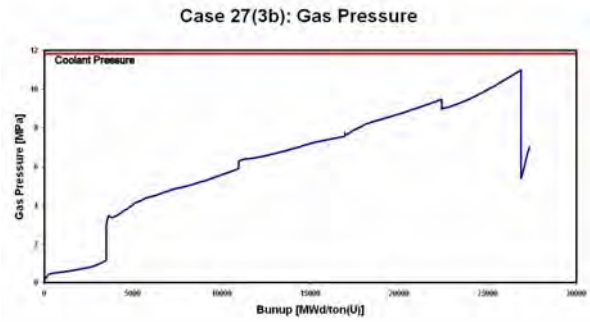


Fig. 3: Internal gas pressure (BaCo, CNEA, Argentina).

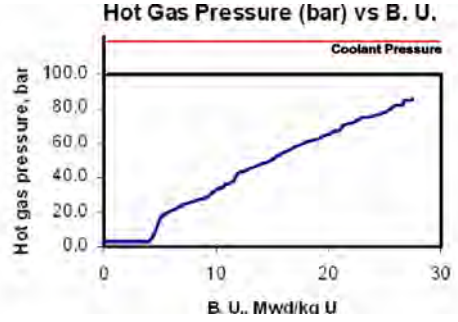


Fig. 4: Internal gas pressure (Profess, BARC, India).

***Example 2: Effect of Power Envelope on Fuel Performance (Case 27 (3b))***

The objective of this experiment was to examine differences among codes related with the effect of envelope power on fuel performance parameters and the sensitivity to coolant temperature and pressure on fuel during irradiation. The main purposes of this exercise were: to verify that the codes continued showing reasonable

trends when element linear ratings changed with time; to identify differences among codes from sensitivity to coolant temperature and pressure; and to analyze the necessary design changes in order to keep the full fuel integrity along the power history. The power history for the second CANDU simplified case was used for fuel design including some power jumps between the nominal design power history and the reference over power envelope. The inner gas pressure was under the coolant pressure value during the irradiation (see Figure 3). The same result was obtained for the Profess code –BARC– (see Figure 4). A low overpressure was calculated for START-3 –VNIINM– and an extreme overpressure for ELESTRESS–AECL– [9].

**Comparison of the Simulation of Indian CANDU Fuel**

A complement of the CRP FUMEX II was carried out with experimental data produced for BARC, India [10]. The fuel of the blind test was a CANDU (a 19 fuel rod bundle irradiated in the Kakrapar Atomic Power Station-I (KAPS-I) up to about 15000 MWd/tonU and subjected to detailed post-irradiation examination (PIE) in the hot cells facility at BARC).

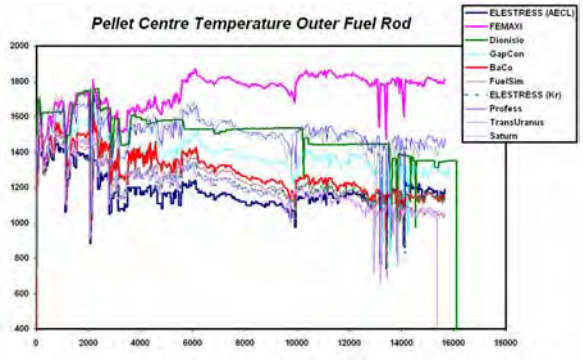


Fig. 5: Code calculations of the pellet centre temperature of an outer fuel rod of the PHWR bundle K1-56504.

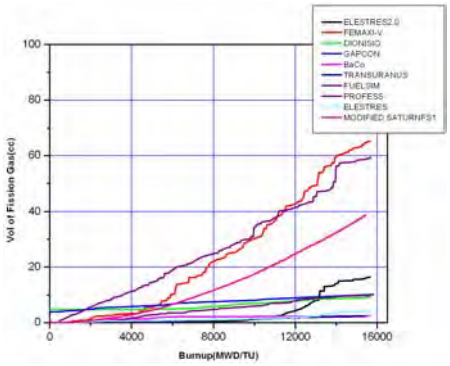


Fig. 6: Code calculations of the volume of fission gas release of an outer fuel rod of the CANDU bundle.

Figure 5 shows the code simulations results related with the pellet center temperature versus burnup for the outer fuel rod. The high temperature of the pellet is a consequence of the big diameter of this type of fuels. The results at the EOL are located in a temperature band width of ~700°C. However, the dispersion is only ~400°C if the top curve is disregarded. The increment of the dispersion started at EOL around to ~4000 MWd/tonU. After that value, the dispersion band remains approximately constant.

Figure 6 shows the volume of the Fission Gas Release (FGR) versus burnup. A great dispersion during the irradiation is observed and an amount of FGR between ~3 to ~65 cm³ at EOL is obtained. A similar behavior was observed for the inner gas pressure and a value of ~5 to ~9 MPa [9] at EOL is obtained. The codes with the maximum of FGR are not the same that the codes with the maximum of pressure. That means a different evaluation of the temperature (see Figure 5) and the free volume in the fuel rod.

This exercise is outdated because it was based on an old CANDU fuel with 19 fuel rods. In fact, the present generation of CANDU fuels contain 37 fuel rods (that means a reduction in the linear power) and the projected CANFLEX and CARA [3] fuels are increasing the number of fuel rods, among others improvements.

**Behavior of Argentinian fuels**

The decrease in the linear power of the fuel rods is due to the increment of the number of rods of the fuel assembly. That is a consequence of the reduction of each fuel rod diameter by keeping constant the total fuel material in the fuel assembly. The first result is a strong reduction of the fuel pellet temperature. The BaCo code simulations show several benefits in the safety and performance of the fuel assembly if the temperature at the pellet center remains below 1400ºC. Those advantages are: no central hole, no columnar grains, decrement of the FGR, less thermal expansion, reduction in the fuel deformations, no plastic behavior in the center region of the pellet, an increment of the pellet cracking with cracks crossing the pellet, increment of the effective pellet radius due to the relocation of pellet fragments, etc. The fuel pellets structure become more uniform but high stresses can be find at the cladding when PCI is attained because a plastic state enough to allow the release of the fuel rod stresses is not achieved in the inner region of the pellet. Those results are among the main findings obtained with the BaCo code when it simulates the expected behavior of the CARA fuel [3] and of the CAREM reactor fuel [4.

**Fuel Behavior under Dry Storage Conditions**

It is usually accepted that the fuel element must not fail during the operation of the power plant. However, it is emphasized in this work that the fuel integrity must also be kept during the intermediate storage at pools or silos. The simulation of the fuel behavior under dry storage conditions can be calculated by using the BaCo code as an extension of the normal application of the analysis of nuclear fuel elements under irradiation. The safe conditions of storage, in particular the temperature of the dry storage system, were analyzed and the results are presented in the Figures 7 and 8. The figures show a stress analysis versus time of two different PHWR fuels during the operation and during the dry storage [14, 15]. We found that there is a small increment of stresses and gas pressure into the fuel rod due to a small fission gas release thermally activated in the presence of the corrosive elements or compounds as I, Cs, CsI, etc. A Stress Corrosion Cracking (SCC) failure could be achieved in the fuel due to the accumulated damage of the cladding during irradiation and the small but constant increment of FGR.

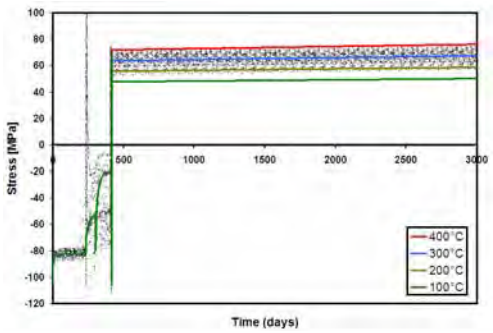


Fig. 7: Hoop stress (tangential stress) at the inner surface of the cladding Atucha I fuel during the irradiation and the dry storage [14]. The cladding is under a traction state. We take into account four different temperatures for the storage. The statistical analysis was calculated at 300°C.

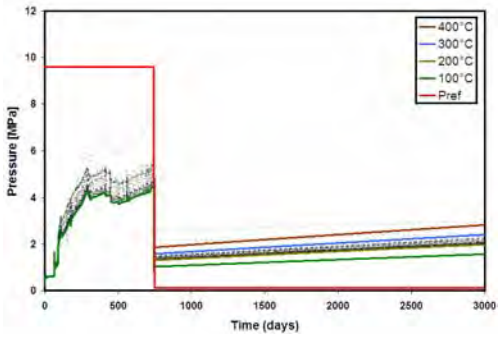


Fig. 8: Inner pressure of the fuel rod due to the free gases of an experimental CANDU (one of the CRP FUMEX III cases) [15]. The red curve is the pressure out of the cladding.

**New Materials and New Fuels with BaCo**

As it was mentioned in the BaCo code description section, the symmetry of revolution adopted for the fuel rod and the modular structure of the code allows us to include new materials for the fuel pellet, the cladding and/or the filling gases. Here we present two examples of the use of BaCo with different fuel materials.

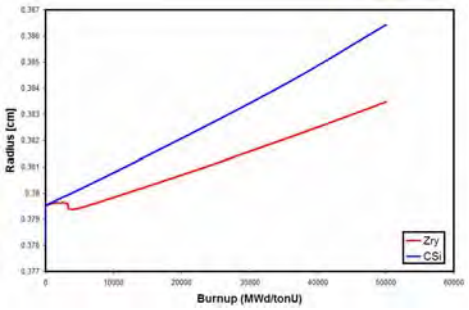


Fig. 9: Pellet radius evolution of two fuel rods with Zry-4 and CSi cladding irradiated in PWR conditions and at constant power.

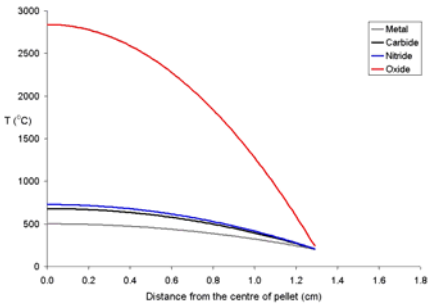


Fig. 10: Fuel pellet center temperature of a 26 mm diameter CANDU pellet with a power density of 250 W per cubic meter.

An approach of the behavior of CSi claddings is summarized. The Figure 9 includes a comparison of the evolution of the fuel pellet radius versus burnup of $UO_2$ pellets by using a Zry-4 cladding and the second rod with a CSi one in PWR conditions. The difference observed in the BaCo simulation results are mainly due to the fact that Zry is a metallic alloy and CSi is a ceramic. The Figure 10 shows the radial profile of the pellet temperature by using different materials for the pellets (metallic U, Uranium Carbide, Uranium Nitride and $UO_2$). It is clearly shown the strong reduction of the fuel temperature when a material with a good thermal conductivity is used. The previous results highlight that the BaCo code is ready to be applied to Generation IV reactors if the fuel has symmetry of revolution.

**TOWARD THE MULTISCALE MODELING OF NUCLEAR FUELS FOR GENERATION IV REACTORS**

There has been a considerable interest in actinide nitrides and carbides during the last years due to the Generation IV reactor initiative. The current experimental database could be enough to support empirical correlations and modeling for current fuels. Nevertheless, as was mentioned in the introduction, 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. The Multiscale Modeling of Materials (MMM) is a new field in Computational Material Science that allows the study of complex phenomena such the behavior of new fuels and cladding materials, and as consequence, could provide a theoretical methodology to obtain the required information. The MMM 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, followed by the development of effective or model potentials to be used in molecular dynamics and kinetic Monte Carlo codes. However, molecular dynamics simulations requires 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 Generation IV reactors.

Although there are several possibilities for developing an inter-atomic potential by fitting the parameters to experimental or theoretical data, the approach followed in this research is different. Mainly, it is an attempt to compute the fcc Th physical and thermal properties through a free-parameter pairwise potential computed from the first-principles calculations of the cohesive energy coupled to the Chen-Mobius lattice inversion method [16]. The cohesive energy was obtained from the full potential LAPW method as it is implemented in the WIEN2k code [17]. The energy curve of fcc Th thus obtained was fitted with the equation of state (EOS) of Birch-Murnaghan to obtain the lattice parameter, equilibrium volume Vo, the bulk modulus Bo and its derivative Bo`. The elastic constants were calculated by applying different strains to the lattice and calculating the resulting energy changes by applying the calculated potential. The calculated lattice parameter, bulk modulus, elastic constants and related magnitudes are summarized in table I and compared to the experimental data [18] and previous theoretical results computed from the phonon spectrum and *ab initio* calculations [19-21].

The elastic constant is one of the most relevant and difficult set of properties to be described accurately and provide valuable information about the binding features between adjacent atomic planes and its anisotropic characteristic. The elastic constants calculations is an important test to any inter-atomic potential and also to *ab initio* method as their calculations require the resolution of small energy shifts that arise when the lattice is slightly distorted. Previous theoretical results show an average error around 8% in Th compared to experiment [18]. The elastic constant obtained in this work are in well agreement with the expected results obtained from a pair potential with an error of 0.3% and 8% for the elastic constants *C11* and *C12*, respectively. The errors are similar or less than previous theoretical results based on *ab initio* phonon calculations. The remaining elastic constant *C44* is too small in our calculations, an expected result if a central potential is used.

Table 1: Physical and thermal properties of fcc Th. *a*: lattice parameter, $C_{11}$, $C_{12}$ and $C_{44}$: lattice constants, B: bulk modulus, G: shear modulus, E: Young modulus, ν: Poisson's ratio, $\theta_D$: Debye temperature and α: thermal expansion coefficient.

| | *Ab initio* | | | | Exp | Potential |
|---|---|---|---|---|---|---|
| | Phonon [19] | FPLMTO [21] | VASP [20] | Wien2k this work | [18] | this work |
| *a* [Å ] | 5.02 | 4.91 | 5.05 | 5.056 | 5.08 | 5.056 |
| B [GPa] | 56 | 63 | 50.01 | 57.1 | 54.3 | 57.1 |
| $C_{11}$ [GPa] | 86.0 | 55.30 | 81.4 | 82.0 | 77.7 | 75.6 |
| $C_{12}$ [GPa] | 39.5 | 35.3 | 40.7 | 40.7 | 48.2 | 44.0 |
| $C_{44}$ [GPa] | 58.4 | 45.9 | 49.5 | 56.5 | 51.1 | 36.6 |
| G [GPa] | | | | | 308 | 283 |
| E [GPa] | | | | | 783 | 723 |
| ν [GPa] | | | | | 0.27 | 0.28 |
| $\theta_D$ [$^oK$] | | | | | 163±3 | 161.7 |
| α [$^oK^{-1}$] | | | | | $11.3x10^{-6}$ | $11.5x10^{-6}$ |

Based on the computed elastic constant and by applying the quasi-harmonic approximation, it is possible to study the thermodynamic properties of Th such as thermal expansion coefficient, Grüneisen parameters, and Debye

temperature obtaining results with an error comparable or less to the results of others works. The results are also presented in Table 1.

The methodology under current development has proven to be very useful also in the determination of the volume dependence of the free energy at a given temperature and the description of the pressure effects. The Pressure vs. Volume equation of state is summarized in Figure 11 and compared with previous theoretical results [20] and experimental data [22]. The agreement between our results and the experiment data is very good.

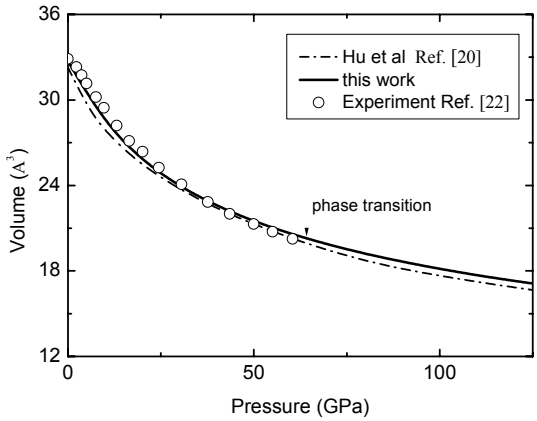


Fig. 11: The static equation of state for fcc Th.

The free-parameter pair potential presented in this work describes with accuracy the mechanical and thermal properties of fcc-Th. However, the next step in our research will be to build an n-body free-parameter potential suitable to be used in molecular dynamic calculations in order to predict the microstructure evolution and atomic site redistribution in fcc Th and multicomponent Th-based nuclear fuel.

## CONCLUSIONS

In this work, the BaCo code was applied to simulate the fuel rod behavior in two selected examples from the IAEA Coordinated Research Project (CRP) on "Improvements of models used for fuel behavior simulation" (FUMEX II). The first test presented in this work was an irradiation computational experiment related with the design of an advanced CANDU fuel. The second one was a comparison between a real experiment of irradiation and the results of BaCo simulations. It is clearly shown the difficulties to obtain a complete set of experimental data in order to cover the development and validation of the fuel behavior modeling. In addition, this work describes briefly the main features of BaCo, as for example: the 3D tools, the statistical analysis, the full core calculations and data post-processing in order to improve the code's performance and the analysis of the results.

The modular structure of BaCo easily allows the inclusion of new models and material properties. Taking into account this advantage, this work present the analysis of the fuel behavior under dry storage conditions and the use of new materials, as CSi, for the fuel cladding and advanced nuclear fuel materials for the pellets, as UN and UC. The condition for performing this analysis is to keep the symmetry of revolution of the fuel (cylindrical fuel rod). 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

Nowadays, the needs for new material parameters could be covered by using the multiscale modeling in order to include new materials and to extend the field of application of the modeling and the code. Actinides nitride and carbide represent examples of the limitation found in the research of new fuel and materials due to the limited experimental information available. The results presented in this work suggests that modeling has reached the point where effective and practical answers can be obtained, becoming a source of experimental information to current relevant problems in Generation IV framework.

This work highlight that BaCo is ready to be applied to Generation IV reactors, if the fuel has symmetry of revolution. The *ab initio* and multiscale modeling can enhance the field of application of the code by including a strong physical basement covering the unavailable data needed for those improvements.

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