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# Multi-scale approach to advanced fuel modelling for enhanced safety

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ABSTRACT

The activities on fuel behaviour modelling using the multi-scale approach, carried out at IRSN and PSI, are described. The perspective of the two organizations on already acquired and potential future advantages from mutual application of the micro-, meso- and macroscopic simulations for fuel reliability and safety is presented. Finally, the conclusion is put forward regarding the merit to further develop the multi-scale approach to fuel behaviour modelling at IRSN and PSI.

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## 1. Introduction

Understanding the thermo-mechanical behaviour of complex systems such as nuclear fuels is more and more based on a detailed description of mechanisms that involve a hierarchy of spatial (from nm to microns) and temporal (from picoseconds to tens of years) scales. In this context, the multi-scale methodology is highly developed in material science. It aims to develop relevant models to describe the interaction between microscopic scale, micro or nanostructure and macroscopic behaviour. This approach requires a good understanding of the theoretical methods (statistical physics, diffusion and rate theories for microscopic-scale objects, as well as macroscopic thermo-mechanics of the continuum materials) and the experimental ones (X-ray diffraction or neutron, local or global mechanical and thermal measurements) used to characterize systems at different scales. The overall objective is to achieve, by building bridges between spatial and temporal scales, the understanding of the macroscopic behaviour of materials. For example, from the nanoscale interatomic interaction description, based on the electronic structure determination with a relevant and possibly adjustable precision, it is possible to identify the basic mechanisms involved in the phenomenon under study at scales less than a nanometre and nanosecond. Then, deducing effective mechanisms (e.g. diffusion), it is possible to move to higher scales (distance and time) and connect the microscopic approaches and continuous approaches (elastic, plastic and creep deformation, fuel material dimensional change, fission-gas release, etc). Finally, the events identified and their characteristics can be used to feed simulation software used to better understand the evolution of "realistic" materials at the macroscopic scale during their entire life. These programs are generally based on approaches of "continuum" type and are based on simplified behavioural models.

As part of study of complex materials, the use of multi-scale approaches became very promising if one wants to be predictive, with a consideration of finer material complexity and required accuracy in the characterization of their behaviour, while the full macroscopic tests are extremely expensive and therefore limited in numbers. If one wants to understand and explain the phenomena governing the behaviour of these materials at macroscopic scale or predict the evolution of their properties, it is essential to exploit data from the microscopic scale and provide feedback to mesoscopic and macroscopic ones. A study at the microscopic scale can not only identify the predominant mechanisms considered at the upper level, but also feed the model with parameters very difficult to obtain experimentally. Indeed, fuel behaviour codes are becoming more accurate and predictive as they are based on increasingly mechanistic models, but assume thereby more parameter to determine and validate. From a scientific point of view, the challenge is multifaceted: first of all, it is to be identified what the relevant phenomena for one macroscopic characteristic, and the scale at which this phenomena must be studied are. Then, the different scales of interest should be connected, making sure

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that the same physical phenomena are not taken into account several times (once effectively hidden in the mesoscopic approach, and a second by an additional term directly from microscopic approaches for example).

The aim of this paper is to outline how this multi-scale approach to the nuclear fuel behaviour simulation has been utilized at IRSN and PSI to improve fuel behaviour modelling.

## 2. Context and scientific method

### 2.1. Macroscopic scale

The objective of the multi-scale approach applied to the study of pressurized water reactor fuel behaviour is to provide modelling tools to simulate the macroscopic behaviour of the fuel throughout its life cycle, i.e. in normal and accident conditions, and also during transport and storage. These tools are essential for the safety analysis and also help to interpret and analyze the full scale experiment results that are available (Studsvik Cladding Integrity Project-SCIP (OECD SCIP Project website, 2015), Cabri International Program-CIP (Cabri International Project website, 2015), Halden Reactor project (OECD Halden Reactor Project website, 2015), Nuclear Science Research Reactor-NSRR program (NSRR page on JAEA website, 2015), etc.). These computer codes, called fuel performance codes, reproduce the macroscopical thermomechanical behaviour of one or more fuel rods. In particular, they calculate the time evolution of temperature, mechanical stresses, deformation and oxidation of the fuel cladding elements based on power levels and thermal-hydraulic conditions (temperature, nature and flow of the coolant), that they are subject to. In general, they also provide information on the behaviour of fission gases (fission gas release, bubble and pore formation and evolution, etc). Currently, most fuel codes, and in particular those used in the field of safety, work with correlations based on the burnup, adjusted on available experimental data. The validity ranges of these models are in fact limited to the experimental data used to define these relationships, and any extrapolation to new materials or new fuel loading schemes is prohibited. In addition, experimental data often present a relatively high dispersion for a given burnup. Indeed, the fuel micro-structure and therefore all its thermomechanical properties can be quite different depending on the irradiation history and the power and temperature to which it was submitted. For example, fuel cracking, fission gas distribution inside the fuel pellet are very closely related to the levels of temperature and neutron flux to which the fuel has been exposed to. Also, the correlations used did not allow for a very accurate modelling of fuel behaviour.

### 2.2. Mesoscopic scale

To meet the above-mentioned challenges and extend the validity domain of the analysis, fuel codes tend to change, and the old correlations were replaced by physical models that explicitly take into account the evolution of the fuel microstructure. Given the very small size of the microstructural heterogeneities compared to the size of the modelled fuel rods, it seems inconceivable at present to simulate directly the microstructural evolution of a whole reactor core. The difficulty is twofold. It is on the one hand to find equivalent behaviour laws for fuel, which allow – from a given microstructural distribution, – to determine the properties of the fuel, and on the other hand, to be able to determine the temporal evolution of the microstructure. On the first point, it is the objective of scaling methods in general and micromechanical homogenization in particular. On the second point, it is solved by the development of new computer codes, called mechanistic codes. These codes are designed to a comprehensive and accurate modelling of all the mechanisms occurring at the mesoscopic scale. They are focused on phenomena taking place at scales ranging from a few tens of microns (the size of a fuel grain) to a few millimetres (a fuel pellet) and of the order of a millisecond up a few tens of seconds. Models are usually based on mean-field approaches. These new computer codes allow on the one hand to explore conditions of operation much broader than those of fuel codes, and on the other hand, they are valuable tools for interpretation and definition of experimental programs, particularly for analytical tests. Finally, they provide a scientific basis for the development and validation of simplified physical models used by macroscopic fuel codes. Another type of modelling approaches allows for studying the evolution of the microstructure beyond the mean-field models: kinetic Monte Carlo approaches, accelerated molecular dynamics, phase field approaches, and dislocation dynamics, for example.

It is important to note that all these mesoscopic approaches requires coupling and that these approaches should not be separated. The mechanical properties, the microstructure, the fission products behaviour, the nature of the phases, all of these are intrinsically interrelated: the microstructural evolution explicitly depends on the temperature and stress which are obtained via the behaviour laws dependent on the microstructural state. Although it may seem tempting to link the microstructural and micromechanical approaches (coupling of a mean-field code and a thermomechanical code for example), such a coupling is complex to implement and could lead to prohibitive computation times. It is therefore appropriate at this time to estimate the relevance of any coupling with respect to a simple chaining or even the use of codes at the lower level to provide more relevant models to the next level as it is currently the case.

All these mesoscopic models are based on microstructural data (fission gas pressure, surface tension, characteristics of the populations involved, and diffusion coefficients). These data can be obtained by two different ways:

- by experimental microstructural characterization techniques such as adsorption microstructural analysis, scanning electron microscopy (SEM), transmission electron microscopy (TEM), wavelength dispersive X-ray spectroscopy (WDS), energy dispersive X-ray spectroscopy (EDS), micro-XRD, and more recently the secondary ion emission spectroscopy (SIMS), elastic recoil detection analysis (ERDA), micro-indentation or tomographic probe. Although more efficient, these approaches do not allow access to all parameters. In addition, the need for these studies on hot cells for nuclear materials greatly limits the amount of available data;
- by simulations at the atomic scale, those describe the interatomic interactions. This description includes the so-called *ab initio* approaches as well as the lighter but parameterized ones such as the tight-binding method which allows for modulating the level of description necessary for the proper treatment of the problem discussed.

These are microscopic simulation approaches that are described below.

### 2.3. Microscopic scale

#### 2.3.1. Needs

As part of the multi-scale approach, the calculations at the atomic level concern nanometric systems for periods of picoseconds to milliseconds. These approaches allow:

- To access the value of parameters needed for mesoscopic modelling (phases identification, solubility, stress calculations

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