Chapter 2.

Nuclear fuel deformation phenomena

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Abstract

Nuclear fuel encounters severe thermomechanical environments. Its mechanical response is profoundly influenced by an underlying heterogeneous microstructure but also inherently dependent on the temperature and stress level histories. The ability to adequately simulate the response of such microstructures, to elucidate the associated macroscopic response in such extreme environments is crucial for predicting both performance and transient fuel mechanical responses.

This chapter discusses key physical phenomena and the status of current modelling techniques to evaluate and predict fuel deformations: creep, swelling, cracking and pellet-clad interaction. This chapter only deals with nuclear fuel; deformations of cladding materials are discussed elsewhere. An obvious need for a multi-physics and multi-scale approach to develop a fundamental understanding of properties of complex nuclear fuel materials is presented. The development of such advanced multi-scale mechanistic frameworks should include either an explicit (domain decomposition, homogenisation, etc.) or implicit (scaling laws, hand-shaking,…) linkage between the different time and length scales involved, in order to accurately predict the fuel thermomechanical response for a wide range of operating conditions and fuel types (including Gen-IV and TRU).

Introduction

Fuel materials used in nuclear reactors are exposed to complex thermomechanical processes during their operation and storage resulting in deformation mechanisms such as swelling, creep, pellet-clad interaction (PCI) and cracking. Fuel deformation is clearly one of the important areas, which requires further understanding and model development for new fuel design and qualification programmes. The traditional experimentally-based paradigm requires several decades of development and is simply not a viable option for evaluating the multiple future fuel candidate designs.

Many of the aforementioned fuel mechanical responses are profoundly influenced by an underlying heterogeneous microstructure but also inherently dependent on the operating temperature and mechanical loading. During in-pile operation, the fuel chemical composition and its microstructure are strongly dependent on high-temperature gradients, neutron irradiation, transmutations and formation of fission products. In turn, these environmental factors affect the fuel chemistry (e.g., electronic excitations modifying the chemical bonds or fission and transmutation reactions altering the chemical composition), the fuel thermomechanical properties (e.g., irradiation creep or fuel cracking) and the fuel microstructure (e.g., nuclear interactions with neutrons and fission products inducing atomic displacements and disturbance of the crystallographic structure; irradiation effects changing and damaging the microstructure). Given these complicated processes, nuclear fuel is constantly transforming during its life (reactor operation and storage), but most of our present understanding and modelling of fuel deformation mechanisms remains empirical, and cannot be easily extrapolated to new fuel compositions, environments, or operating conditions. This is partly due to the fact that basic underlying mechanisms governing swelling, creep, PCI and cracking for this complex material remain for the most part poorly understood.

Figure 1 shows the results of a PIRT (Phenomena Identification and Ranking Table) process for identifying key phenomena associated with fuel deformation [12,81]. Both normal and abnormal situations are included in this figure. These phenomena are ranked based on both their importance and the current state of knowledge. What Figure 1 intelligibly shows is that items located in the upper right corner are the ones with the most impact per resource allocation on fuel deformation. It clearly appears that the most influential features are in fact associated with fission products, irradiation effects and fuel microstructure evolution.

As it will be discussed in the following of this chapter, numerous investigations have been conducted over the past 20 years and various mechanistic codes and models (mostly continuum) have been developed in an attempt to address and study fuel mechanical behaviour under various conditions (steady or transient). Table 1 summarises a brief list of representative mechanistic codes and their application. These codes generally consist of three main components [3]:

- a thermal analysis part dealing with the temperature distribution and the inventory of fission products within the fuel;

- a mechanical analysis part treating the mechanical interaction between pellet and cladding, and the stress and strain state in the fuel pellet and cladding;
- a material properties section referencing materials property libraries.

Figure 1. PIRT

System	Operational or design issue	Phenomena to be controlled	Mechanism to be understood
LWR	Under normal operating conditions : limitation of pressure inside the rod	Fission gas release Swelling (gaps collapse)	Fission gas transport and precipitation
	Under accidental conditions : limitation of the fission gas release	High burn up structure formation that can lead to large fission products release and actinide dissemination	Effect of irradiation on microstructure/ transport of constitutive elements and solid FP's
HTR	Under normal conditions : limitation of mechanical loading of the coatings and FP's escape	Fission gas and CO pressure in the particles Chemical interactions between FP's and coatings elements	Fission product speciation in UO2 kernel and coatings
GFR	Know the operating limit temperature of U and Pu carbide fuels	Carbide dissociation/Pu vaporisation	Thermo chemical stability through phase diagram calculations
	Prediction of fuel element geometrical changes	Swelling of carbides	Irradiation damage/fission gas transport and swelling porosity/creep
SFR	Know the operating limit temperature of oxide fuels containing minor actinides	Thermo chemical stability of oxides with minor actinides	Impact of minor actinides on phase diagram/ actinide and O redistribution
	Control chemical interaction between fuel cladding and thermal bond	FP's compounds formation near the cladding	Thermo chemical stability of FP's compounds. FP's migration in the pellet
All fuel types	Under accidental conditions, limit the source term	FP's release and fuel behaviour	Thermo chemical stability of FP's compounds/FP's migration in fuel and coatings/swelling/creep

All these codes present diverse models with various degrees of refinement for the evolution of a variety of microstructural descriptors ranging from intragranular fission products transport to grain growth. The general strategy adopted for these codes is to lump various characteristics of the microstructure into effective properties or empirical laws and solve a set of coupled differential equations describing the coupled physics of the system. Although these codes are reasonably successful in predicting the fuel mechanical response where the empirical correlations are valid, as it was pointed out in the above, this response is impacted by sub-continuum phenomena. Improvements in this modelling approach are possible and require lower length scale modelling tools. These models span all time and length scales starting from the nuclear and electronic structure, to the atomistic and grain level and finally to the continuum level. Figure 2 illustrates this multi-scale paradigm. Such an approach brings further fundamental insight into the understanding of the physical, chemical and mechanical behaviour of nuclear fuel under various conditions (high temperatures and irradiation).

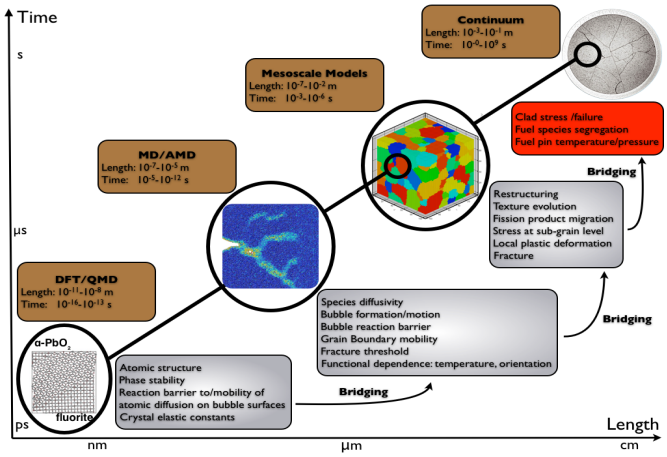
This chapter seeks to demonstrate the capabilities and challenges associated with modelling nuclear fuel deformation, both in terms of the current state-of-the-art and on-going efforts to improve predictive modelling capabilities. In particular, in the reminder of this chapter, we will review various aspects of fuel mechanical deformation (creep, swelling, cracking, and PCI) in terms of the different mechanisms and physical

phenomena involved and their relevance. The status of current modelling strategies and on-going efforts for each of these deformation modes will be discussed. We will conclude this chapter by presenting future perspectives and research needs for the characterisation and modelling of thermomechanical response of nuclear fuel. Note that this chapter deals with the deformation of fuel materials only. Deformations of cladding materials are discussed elsewhere.

Table 1. Representative mechanistic codes for fuel mechanical behaviour and their application

Code	Application	Reference
BISON	Performance for light water reactor	Newman (2009) [48], Williamson (2011) [80]
AMP	Performance for oxide fuel in a light water reactor or metal fuel in a sodium-cooled fast reactor	Philip (2010) [56], Turner (2009) [72]
MFPR	Performance for light water reactor	Veshchunov (2006, 2009) [76,77]
FRAPCON	Performance for light water reactor	Berna (1997) [7]
FRAPTRAN	Transient behaviour for light water reactor	Cunningham (2001) [18]
FEMAXI-6	Performance and transient behaviour for light water reactor	Suzuki (2004) [69]
TRANSURANUS	Performance and transient behaviour for light water reactor	Lassmann (1992) [34], Van Uffelen (2008) [74]
ELESTRES	Performance code for CANDU fuel	Tayal (1996a,b) [70,71]
LIFE	Performance for fast breeder reactor	Jankus (1972) [30]
PLEIADES/ALCYONE	PWR: Nominal; transient and accidental behaviour	Sercombe (2009) [65], Sercombe(2010) [66], Marelle (2011) [39], Struzik (2012) [68]
PLEIADES/GERMINAL V2	SFR : Nominal; transient and accidental behaviour	Lainet (2011) [33], Bouineau(2011) [11]
PLEIADES/MAIA	MTR : Nominal and transient behaviour	Marelle (2007) [38]
PLEIADES/ATLAS	HTR&VHTR: Nominal and transient behaviour	Michel (2006) [41]

Figure 2. Paradigm of multi-scale modelling for nuclear fuel mechanical behaviour



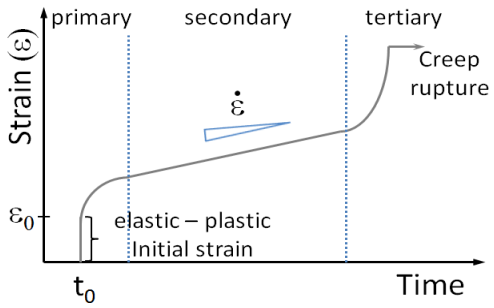
DFT: Density Functional Theory (*ab initio*), QMD: Quantum Molecular Dynamics (electronic structure), MD: Molecular Dynamic (atomistic), AMD: Accelerated MD (atomistic), Mesoscale models: grain-level techniques such as Monte Carlo, Phase Field, Mean Field, Continuum: Finite Element-like techniques.

Creep

In material science, creep defines a slow irreversible deformation process under the influence of stresses below the yield stress and has various origins, mechanical, thermal or irradiation. It must not be confused with plastic deformation, which relates to an instantaneous process. In a reactor, thermal creep and irradiation creep produce dimensional changes of the fuel element which can lead to severe deformation and reactor accidents. For long storage times even if the fuel temperature drops additional pressure may appear due to the increase of fissions gas products. For instance, for UO_2 fuel the additional pressure could be 1 MPa and 2 MPa after 100 and 300 years, respectively. For MOX fuel, which contains more α emitters, the helium pressure could be significantly higher: 7 and 12 MPa after 100 and 300 years [59]. Moreover, the temperature range is rather large and the duration that one needs to consider is much longer. Therefore, for reactor material design and safety assessment, creep is an important phenomenon that needs to be addressed and modelled.

With time, creep evolution is usually divided in three different stages (see Figure 3): (i) the primary creep presents high amplitude plastic deformation with strain rate that continuously decreases, (ii) the secondary creep or stationary creep is the stage where the strain rate is constant, and (iii) the tertiary creep relates a rapid increase of the strain rate during which the material is strongly degraded and leads to its failure.

Figure 3. Schematic representation of strain as a function of time due to constant applied stress

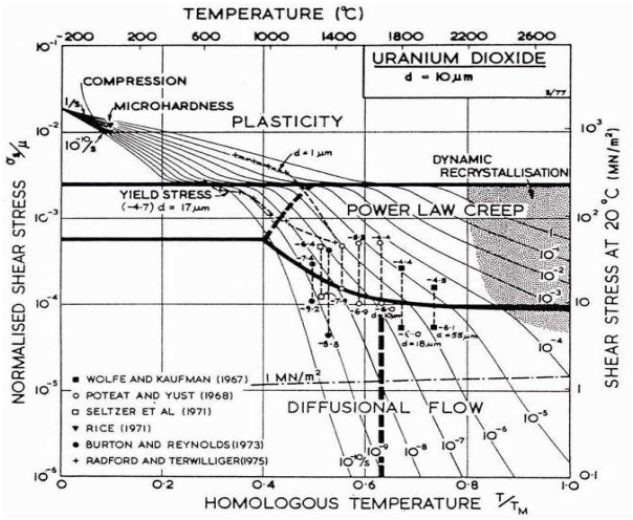


The primary creep corresponds to a small fraction of the total creep but it contributes more to the total strain at lower temperature and can play an important role on the fuel behaviour in pile during transient event. However, it was very little studied because of the experimental set-up difficulties and the absence of theoretical model. The secondary creep is the most important regime both in terms of time and accumulated strain and often the only one considered in an engineering assessment. Tertiary creep constitutes generally a very short time and therefore can often be neglected.

To summarise the creep behaviour in UO_2, Ashby et al. [2] have gathered all the data available at the time in a data map (see Figure 4). This map gives a good overview of the deformation mechanisms, which take place in UO_2 during creep. It defines the temperature range at which the different mechanisms are predominant. This map shows that creep is greatly dependent on temperature. Below temperatures 0.4 T_m (1 000°C for UO_2), the material is highly resistant; none or almost no permanent deformation has been measured below the

yield stress. This behaviour is common for most of the oxide materials. Above 0.4 T_m, the oxide creeps with two different regimes according to the level of applied stress, which are separated with a threshold stress noted in the following σ_t. At the higher stresses, creep rate follows a power law, which is generally related to a dislocation diffusion mechanism. At lower stresses, creep rate is controlled by cation diffusion and follows a linear diffusion flow law.

Figure 4. Stress/temperature map for UO_2 with grain size of 10 μm [2]



To be used for engineering purpose, creep models need to be treated at the continuum level (macroscopic scale). From the standpoint of the continuum representation, solution of the creep problem requires statement of the mechanical equilibrium equations, appropriate constitutive equations for creep behaviour and suitable initial and boundary conditions. A commonly used equation of state representation for primary and secondary creep is provided by the Bailey-Norton law:

$$\dot{\varepsilon} = A(T)\sigma^n \exp(-E_a/k_B T)$$

where $\dot{\varepsilon}$ is the creep rate, A a material parameter that depends on the temperature T, σ the applied stress, E_a the creep activation energy, and k_B the Boltzmann constant. At applied stresses lower than σ_t, the exponent n, is close to 1, this corresponds to the diffusion flow regime. At applied stresses higher than σ_t, the exponent ranges from 4 to 7 implying that creep rate is greatly influenced with the applied stress. The creep response of materials is intimately related to microstructural processes that take place inside the material during deformation. These processes are included in the parameter A, which depends on the departure to the stoichiometry, the grain size, the density, and the fission products. Therefore the challenge for modelling is to describe accurately this parameter A.

In the literature, various models [37] have been proposed, however, they all have their restrained domain of application. One way to tackle this difficulty is to have a better knowledge of the physical phenomena involved in creep processes at the microscopic level, which could be approached with different modelling techniques. Table 2 summarises the different physical phenomena involved in creep processes and the modelling techniques with which they are susceptible to be treated.

To our knowledge, few simulations dedicated to creep have been carried out at the microscopic scale. We can acknowledge some work on grain boundary effect [20,50], on dislocation [19,22,52], on diffusion at high temperature [32,26,54], on migration of fission products in the fuel [82,29] [36,63,79], and lattice damage caused irradiation [40,73]. Furthermore, most of the experimental studies available were carried out more than 30 years ago. In the following, we will list the issues that are currently under consideration or that still need to be modelled:

- Influence of stoichiometry: The creep activation energy is very sensitive to the evolution of the stoichiometry [62,64]. An excess of oxygen atom increases significantly the plastic deformation of UO_2 and hence increases the creep rate. The value of the threshold stress σ_t depends also on the stoichiometry because of the cation diffusion change with stoichiometry [13]. However, the cation diffusion coefficients are still imprecise.

- Influence of grain size: For stresses lower than σ_t, it is generally admitted that the creep rate is inversely proportional to the square of the grain size [1,10,13]. Conversely, for high stresses, the study carried out by Burton et al. [13] shows an increase of the creep rate with an increase of the grain size. The authors believe that the grain boundaries are acting as sliding barrier, which hardens the material (Cobble creep). No calculation of the grain boundary motion has been carried out yet. However, for big grain sizes, creep is dominated by dislocation motion even for low stresses (Nabarro-Herring diffusion). There is still some controversy about the influence of the grain size on the creep activation energy.

- Influence of density: Several studies [10,27,45] show that the creep rate increases with an increase of the porosity. However, the effect of the pore shape as well as the porosity self-healing intra- and intergranular have not yet been quantified and these parameters are not included in the creep models currently used.

- Irradiation effect: Several studies [16,23] show that creep appears at low temperatures (700-800°C) under irradiation. However, the microscopic physical phenomena behind this behaviour are not yet completely understood. It has been shown that creep decreases if the irradiation with heavy ions increases [17]. Conversely, older studies [55] carried out on spent fuels show that creep rate increases as the burn-up increases. Furthermore, the grain size effect has been studied on creep induced by irradiation but no clear effect arises from these studies [15]. More fundamental knowledge on irradiation effects is still needed to develop accurate model in order to embrace all the effects mentioned above.

- Irradiation effect – Fission products: The fission products as isolated defects or as precipitates reduce the fuel creep [1,9,27]. It is believed that the fission products at the grain boundaries disrupt the diffusion processes. The few available experiment data at high stresses are not sufficient to conclude if dislocation motion is affected by the presence of fission products.

Table 2. Available tools to study key physical phenomena involved in the mechanical response of nuclear fuel

Physical phenomenon	DFT	MD	Meso	Exp	PIE	CAL
Fission products	✓					
Point defects formation/diffusivity	✓	✓	✓			
Clusters of defect formation		✓	✓			
Dislocation loops formation/motion		✓	✓			
Grain boundary motion		✓	✓	✓	✓	
Fuel densification		✓	✓			
Fission gas bubbles nucleation / growth		✓	✓			
Recrystalisation		✓	✓		✓	
Phase transformation/stability		✓	✓	✓	✓	✓
Fission product's solubility	✓					✓

DFT: Density Functional Theory (*ab initio*), MD: Molecular Dynamics (atomistic), AMD: Accelerated Molecular Dynamics, Meso: Mesoscale modelling (grain-level techniques such as Monte Carlo, Phase Field, Mean Field, Dislocation Dynamics), Exp: Experiments, PIE: Post-Irradiation Examination, CAL: CALPHAD thermodynamic method.

Swelling

Accurate estimation of the dimensional changes of ceramic fuels during irradiation is of the utmost importance in predicting the mechanical performance, especially for fast reactor fuel elements. Fuel swelling is mainly due to replacement of heavy metal atoms by fission product atoms. Most of the fission products are solid and their contribution to swelling is commonly considered negligible. However, fission gasses are treated separately because they usually coalesce into bubbles within the fuel due to their very low solubility (Xenon, Krypton) and hence impact significantly fuel swelling.

Many individual physical processes contribute to the behaviour of fission gases in nuclear fuels. Each of them is important and needs to be understood in order to model correctly fuel swelling. We list in the following these behaviours and the attempts that have been achieved with different simulations techniques:

- Nucleation of gas bubbles. Either homogeneously by chance encounters of wandering gas atoms or heterogeneously on fission-fragment tracks or dislocation lines. Several atomistic simulations [46,25] but the full picture.
- Growth of gas bubbles by atomic migration of fission gas atoms to existing bubbles. Bubble growth can be affected by the availability of vacancies to permit the bubble to expand as gas is accumulated and by the effects of surface tension and the stress state of the surrounding fuel matrix, which determine the stable size of the bubble [47,35].
- Re-solution of the gas atoms in the matrix [51,63,24].
- Migration of the bubbles, either as a random-walk process in the absence of directed forces acting on the bubble or as biased motion when such forces are present. The forces that act on gas bubbles in solids are generally believed to be

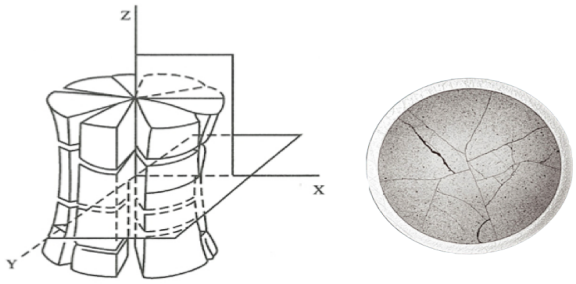
those due to the temperature or stress gradients, or restraining forces due to dislocations and grain boundaries [21].

- Coalescence of bubbles moving either in a random or directional fashion. Only very recently mesoscale simulations have been carried out in this topic [44].
- Interaction of bubbles with the crystal defects (dislocations and grain boundaries). To our knowledge no simulations were done on this topic.
- Release of the fission gases, either to external surfaces such as the central void, cracks in the fuel or the fuel-cladding gap or to internal surfaces such as grain boundaries. Most of the simulations have been done at the mescoscale or in fuel performance codes [48,28,67,53].

Cracking

Cracking of nuclear fuel has a direct impact on the release of fission products and thermal conductivity both during normal and abnormal operational conditions but also when spent fuel is used as the final disposal form. Indeed, a network of cracks increases the surface area of the fuel which, in turn, increases the rate at which fission products can leave the fuel and change thermal conductivity conditions. As such, cracking is an essential secondary phenomenon impacting important properties of the fuel. Immediately after the fuel rod power increases and before any significant swelling or creep can occur (see Section Creep and Swelling), a network of cracks due to thermal stresses is induced by the radial high-temperature gradients (a few hundreds Celsius per centimeter) [49].

Figure 5. Cracking of fuel pellet (a) schematic of a fuel pellet with a "hourglassing" shape due to the effect of thermal stresses, (b) macrograph of a PWR fuel pellet cracked by the thermal gradient [4]



(a) (b)

As shown in Figure 5, these cracks are either oriented along radial planes passing through the fuel-pin axis (sometimes called θ cracks) or along horizontal planes perpendicular to the pellet axis (z cracks). Fracture orientations originate from the thermal stresses generated by the temperature gradient that exist between the centre (1 200^{0}C) and the outer part (400-500^{0}C) of the pellet. Pellet fragmentation during nominal loading is mainly characterised by radial and axial cracks. A second set of cracks appears during the power ramps (transient loading). Three-dimensional simulation of secondary crack network development is now possible with some fuel performance code [42]. The orientation of these secondary cracks is very similar to that of the primary cracks. The parabolic temperature gradient in the fuel induces tensile stresses in the radial and axial directions in

the outer region of the fuel where the fuel is brittle. In the inner core of the fuel, the thermal stresses are compressive, and therefore no cracking occurs inside.

As explained just above, because of high thermal gradients within the pellet, internal thermal stresses are developing in the fuel. These internal stresses can be evaluated by means of numerical methods (finite elements for example) but a good approximation can be obtained with an analytical solution. With the assumption of constant thermal power, thermal conductivity and thermal expansion coefficient, maximum tensile stresses $\sigma_{\theta,max}$ are located at the pellet surface and are:

$$\sigma_{\theta,\max} = \frac{E_\alpha}{2(1-\upsilon)}(T_c - T_S)$$

where E is the fuel Young's modulus, α is the coefficient of thermal expansion, ν is the Poisson's ratio, T_c is the centreline temperature, and T_S is the temperature at the surface of the pellet. If one assume that UO_2 is a brittle material (at least for temperatures below half of the melting temperature), the fuel pellet will crack when $\sigma_{\theta,\max}$ exceeds the ultimate strength of the fuel $\sigma_{\theta,\mathrm{frac}}$, i.e.:

$$T_c - T_S = 2\frac{1-\upsilon}{E_\alpha}\sigma_{\mathrm{frac}}$$

Note that the ultimate strength can vary notably according to the surface quality. For example, if one assumes that the average strength of a typical oxide fuel is about 130 MPa, one would find that the fuel pellet starts to fragment when $T_c - T_S > 100°\,\mathrm{C}$, i.e. during the first power increase to nominal conditions.

In addition, the fuel pellet is subject to thermoelastic deformation. This is due to the fact that the pellet has a finite length (between 10 and 14 mm). It can be shown that under the effect of thermal stresses, the pellet initially orthocylindric tends to a hourglassing shape with convex faces. This means that the approximation of plane deformation is not valid anymore in the vicinity of the pellet faces: the axial stress becomes zero on these faces and this behaviour needs to be corrected in the mesoscale models.

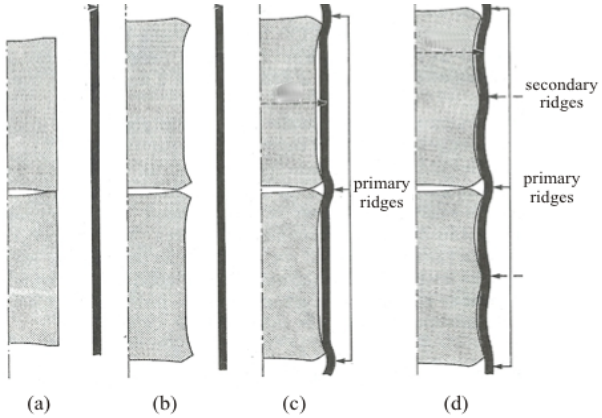
Furthermore, almost all the finite element codes take for approximation that the mechanical properties of the fuel are isotropic and assume that it is a brittle material. However, recent atomistic simulations [84] show that UO_2 can undergo phase transformation at the vicinity of the crack tip corresponding to a more plastic mechanical behaviour. Moreover, irradiation effects on the mechanical properties are seldom included in mesoscale model because they are not fully understood. More investigations in these two topics are then necessary to improve fuel cracking modelling.

Mechanical deformation in pellet-clad interaction

Nuclear fuel rods are fabricated with an initial pellet-cladding gap to offer space for radial thermal expansion and fission product swelling during operation. Pellet-clad interaction is a common fuel failure mechanism caused by fission-products (such as iodine and cadmium) induced stress corrosion cracking (SCC) of the cladding. At the beginning of irradiation, the clad is subjected to a differential pressure between the coolant pressure and the internal gas pressure leading to a compressive state. As illustrated in the schematic of Figure 6, the gap between the pellets and the clad progressively closes down (generally

between one to three years of burn-up, depending on the fuel type) under the combined effect of creep in the cladding material and swelling induced by the accumulation of fission products in the fuel pellet. As a consequence of the typical hourglass shape of the pellet, the first contact between the clad and the pellet occurs at the pellet-pellet interface where the gap is the smallest. Subsequently, the cladding will continue to deform in response to this non-uniform interaction to eventually take the exact shape of the hour-glassed pellet. This mechanism, known as *bambooing*, has been correlated with primary circumferential ridges identified on the cladding diametric measurements after irradiation (see Figure 6(c)).

Figure 6. Evolution of the gap between the cladding and the fuel pellet during irradiation (a) start of irradiation, (b) first cycle and start of second irradiation cycle, (c) second half of second cycle: first cladding-pellet contact and appearance of primary ridges, (d) in the case of power ramp: appearance of secondary ridges [4]



While the gap closes, the cladding, initially loaded in compression due to the high coolant pressure, progressively gets in contact with the pellet and becomes loaded in tension. This tensile state of stress increases slowly to a stress level of about 20 to 30 MPa [6]. Therefore, in nominal conditions, the cladding material can easily accommodate the pellet swelling kinetics: the cladding is loaded by low PCI. During transients (power ramps), the thermal gradient increases rapidly and reaches within a few minutes a value almost three times higher than the nominal value (1 200^{0}C over 4 mm in radius). The corresponding pellet swelling leads to high tensile stresses in the cladding, which cannot easily accommodate by viscoplasticity and can potentially result in the failure of the clad.

In addition, due to the high temperatures, the fuel viscoplasticity is also activated in the pellet centre and leads to a progressive filling of the transversal cracks. The fuel creep is correlated with the formation of secondary ridges at the median pellet plane level (Figure 6(d)). In such strong PCI conditions, the mechanical state of the pellet-cladding system is no more governed by the pellet deformation alone. In fact, the stiffness of the fragmented pellets and the cladding are not so different anymore and the strong cladding mechanical pre-stressing contributes to unbend the fragmented pellets.

The behaviour of pellets in their interactions with the cladding depends on many mechanisms potentially activated prior to or during PCI, namely:

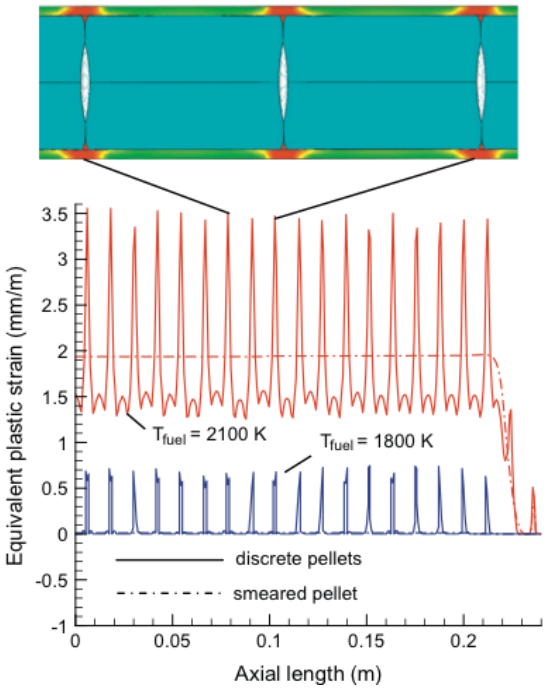
- swelling of solid and gaseous fission products due to burn-up;
- release of fission gases and volatile species;
- evolution of high-burn-up structure (HBS);
- evolution of thermal conductivity, elastic constants, thermal and irradiation creep, temperature-induced or microstructure-induced phenomena (porosity, recrystallisation);
- radiation damage;
- geometry of the pellets and their modifications by cracking;
- formation of contact materials or bonding layers at the interface of the fuel and the clad (zirconia/uranate compounds);
- oxidation, hybridation;
- pellet-cladding interfacial friction.

The present state-of-the-art in modelling PCI predominantly involves modelling the fuel and clad as a single rod representation of the reactor core in an axisymmetric, axially-stacked one-dimensional (1D) representation with few examples of two-dimensional (2D) [61] and three-dimensional (3D) [6,58,43,48,80] simulations. The best known codes are FRAPCON [7] and FRAPTRAN [18] steady-state and transient codes, respectively, used by the Nuclear Regulatory Commission in the United States as audit codes. Industry codes include COPERNIC by AREVA [8], TRANSURANUS by ITU [34,74], or ENIGMA by British Energy [31]. In all the listed codes, the fuel rod is represented and meshed as a continuum divided in four domains: (i) the fuel pellets, (ii) the cladding, (iii) the fuel-cladding gap, and (iv) the cladding-coolant interface. The physical phenomena and processes affecting PCI and described above (at least part of them) are implemented with various degrees of details as correlational (with respect to experimental data) or empirical models and added to the set of equilibrium equations. The thermomechanical solutions representing the interaction between the clad and the pellets are obtained by time splitting the physics and a series of time marching iterative calculations in which the temperatures are calculated in both the pellets and the cladding (based on neutronics) followed by calculations of the state of stress and strain in the pellets and cladding (based on more or less refined constitutive models). The fidelity of the fuel constitutive model greatly influences the heat conductance within the pellet and across the pellet-clad gap which, in turn, affects the gap opening status and PCI contact pressure conditioning PCI failure. Inputs to these calculations are the power history (heat source) and the fast neutron flux and fluence (radiation damage).

For example, Newman et al. [48] from Idaho National Laboratory developed a 2D/3D fuel performance analysis capability (named BISON) which solves the fully coupled thermomechanics and mass diffusion equations, for both steady and transient regime. Implemented as a sub-routine in ABAQUS, this continuum code includes UO_2 temperature and burn-up dependent thermal properties, solid and gaseous fission product swelling, fuel densification, fission gas release, cladding thermal and irradiation creep, cladding irradiation growth, gap heat transfer, and gap/plenum gas behaviour during irradiation. As shown in Figure 7, comparisons between discrete and smeared-pellet

simulations reveal the importance of a multi-dimensional, multi-pellet, fully-coupled thermomechanical approach as opposed to 1D traditional/legacy codes lacking these features. Another example is the EPRI 2D fuel performance code Falcon [61], which computes the thermal, mechanical and chemical behaviour of a single fuel rod during irradiation. Similar to BISON, this continuum code includes empirical models for fission gas release, burn-up, fuel cracking, cladding and fuel viscoplasticity, densification and swelling. Of interest, this code was used to study PCI failure due manufacturing-induced missing pellet surface [60]. As shown in Figure 8, stress distribution predictions in the cladding obtained from these simulations appear to trace the crack propagation path seen in fuel rod failures where missing pellet surface is present.

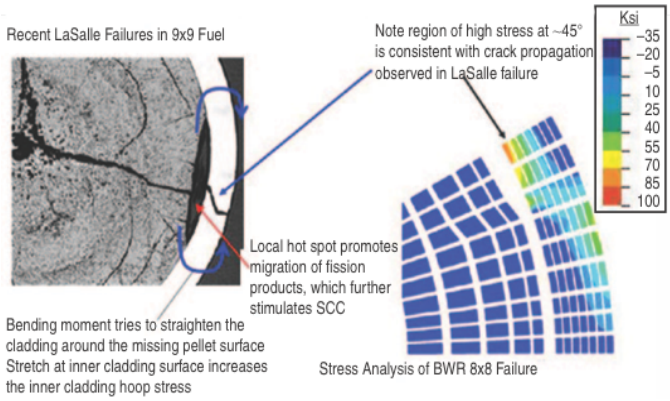
Figure 7. Clad mid-wall equivalent plastic strain, versus axial length, at two centreline fuel temperatures during the power-ramp



Results from both the discrete and smeared-pellet calculations are shown for comparison [48].

Regardless of the progresses made in recent years in the capabilities of these fuel codes where the empirical correlations are valid, these codes remain continuum representations of the fuel rod behaviour despite the fact that PCI is influenced by physical phenomena of several orders of magnitude smaller both in space and time. As such, higher resolution simulation techniques have been recently used to model lower length and time scales processes. These techniques include Density Functional Theory (DFT) and Molecular Dynamics. These atomistic-based modelling methodologies can be used to explicitly provide kinetic behaviours, including the probability of certain events like diffusion and alloying and capture mechanisms that cannot be resolved by coarser theories. Some of these processes are: migration of fission products in the fuel [29,36,63,82], lattice damage caused by fission products and neutron during irradiation [73,40], or the thermal conductivity of fuel pellets [5,57,79].

Figure 8. Manufactured-induced missing pellet surface-induced failure pattern compared to calculation in falcon evaluating cladding hoop stress distribution [60]



The following articles illustrate the use of lower length scale modelling combined with theoretical understanding to improve empirical models of various properties of the fuel. For example, an opportunity has been shown to study the thermal conductivity using MD and show and quantify the variation of the thermal conductivity of UO_2 due to thermal and radiation effects [57]. Ichinomiya et al. [29] studied the migration dynamics of oxygen point defects in UO_2 using temperature-accelerated dynamics simulations giving insight into the formation mechanism of high-burn-up restructuring, including planar defects and grain subdivision (the rim structure), found in UO_2.

Clearly, integrating atomistic and mesoscale simulations results either by informing and improving empirical physical models or by substituting them would greatly benefit PCI modelling. Lower length scale simulations can help identify and inform key physical parameters influencing PCI such as diffusion coefficient used in fission products migration, defects/vacancies mobility or thermal conductivity. More importantly, the development of a multi-scale framework to study PCI would provide the following incentives:

- establish a basis for understanding fundamental phenomena;
- rank their relative importance;
- allow a credible prediction of PCI onset and demonstration of a safe operation of the fuel in-core when validated;
- define relevant experiments.

Conclusions and future challenges

One of the very important issues for the sustainability and the safety of the nuclear reactor is the knowledge of the nuclear fuel physical integrity. Fuel deformation is a complex problem, which includes several physical phenomena at different length and time scales. Therefore, modelling such behaviour involves the use of multi-scale and multi-physics approach with adequate bridge between the different scales and technics. Four key physical phenomena have been identified with their own on-going investigations:

- Creep is a long-term behaviour process, which is very difficult or impossible to study fully via experimental studies. Therefore, modelling and simulations are required. To this day, several models have been proposed but they all have their restrained domain of application. Furthermore, some fundamental knowledge on the stoichiometry and the irradiation effect including fission products on the mechanical properties are still needed to develop more accurate models.
- Fuel swelling is mainly due to the accumulation of inert gas bubbles. A lot of effort has been done in comprehending the nucleation and the growth of those gas bubbles and the fission gas release. However, data on the bubble migration and their interaction with extended crystal defects such as dislocations and grain boundaries are still missing.
- Concerning the fuel cracking and the mechanical deformation in pellet-clad-interaction, several codes in finite elements exist and predict correctly the main crack propagation behaviour seen in fuel rod failure and fuel cracking. However, the evolution of the mechanical properties under high burn-up or accidental conditions is still not fully understood. Insights from atomistic and mesoscale simulations on the lattice damage caused by irradiation or thermal conductivity evolution will provide useful understanding, which will improve the predictability of PCI codes.

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