Challenges in the field of materials science

M. Defranceschi*

The development of innovative thermonuclear fusion and nuclear fission reactors critically depends on the availability of not only nuclear fuels but also advanced structural and functional materials systems. These have to withstand extreme conditions: high temperatures, intense neutron irradiation, and strongly corrosive environments, in combination with complex loading states and cyclic loading histories. The challenges in the field of nuclear materials range from operation in critical conditions to compliance with the highest levels of safety and protection, while giving due regard to decommissioning, dismantling and waste processing issues.

Searching for new materials and tailoring them to the desired multifunctional properties is central to many industries but the nuclear sector must deal with the specific condition of radiation. Hardly any industry escapes having to investigate materials science; practically none must investigate to such an extent as does the nuclear industry. Beyond the sole scientific and technological questions are economic and societal issues: service life extension of nuclear power plants and more stringent safety requirements are increasing the demand for better control of the ageing of materials, components and structures.

Operating conditions offer further complexities. Very severe operational constraints and the extremely high requirements to be able to correctly forecast material behaviours on a long-term basis whereas radiation, thermo-mechanical loading and chemical attacks all combine to severely impair their states. In many respects the understanding gained remains empirical and cannot be easily extrapolated to new materials, new environments, or new operating conditions; basic underlying mechanisms governing manufacturing, behaviour and performance require greater understanding and call for in-depth investigation.

So-called "nuclear materials" are multiple and varied – metals and their alloys, polymers, glasses, ceramics – and can be used in various applications:

Fission: ferritic steel (RPV), austenitic stainless steel (internals), zirconium alloys (fuel cladding), oxide matrices (used fuels).

Fusion: ferritic/austenitic steels (wall and piping), ceramic composites.

Generation IV: iron-chromium alloys, silicon carbide, etc.

Waste conditioning: glasses, cementitous materials, mineral matrices.

Components of nuclear plants: polymers (cable and coatings).

Technological needs

Technological needs vary enormously: which type of materials, which property, which scale of length or time. Key differences between the science of condensed matter or solid state physics and materials science stem from its crucial technological drivers. These cover any assessment of the effectiveness of the design of the material properties, as for example: fitness for purpose (intrinsic property such as the capability to sustain high temperatures), whole life behaviour (e.g. the creeping of materials at high temperatures, the breakdown of polymers under electrical stress, the decomposition of glasses

Dr. Mireille Defranceschi (mireille.defranceschi@oecd.org) works for the NEA Data Bank.

after disposal and the adaptability of materials to new nuclear fuel characteristics as fuel evolves), customer acceptability, economic, safety and environmental aspects (optimising materials for radioactive waste disposal, increasing lifetime).

The challenges faced by materials scientists in the nuclear field are multiple:

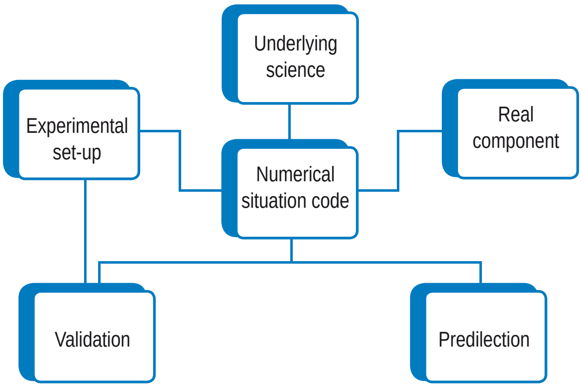
- Nuclear materials science examines multi-component, multi-phase problems, made more complex by variations in scale. The length scales range from atomic to mesoscopic (typically from a few nm to microns) to macroscopic, with these scales sometimes extensively mixed. The timescale ranges from femtoseconds to tenths of years for vessel lifetime to geological timescales for radioactive waste repositories.
- The basic phenomena controlling the behaviour of materials under irradiation are complex. A question still unanswered is: which scale is relevant for the phenomenon? Is it the atomistic scale of electronic structure or is a collective effect occurring at a larger scale? Physicochemical properties of nuclear fuel are important to evaluate too. However there is limited information on these properties due to the difficulties associated with observing high radiation fields.
- Many systems are prepared or used when neither in thermodynamic equilibrium, nor homogeneous; considering them in an equilibrium state is thus insufficient. For instance it is safely admitted that at high temperature most solids are in thermodynamic equilibrium state. At low temperature this is not always true since their relaxation time scales can be very long. A system can also be maintained in a non-equilibrium state exposing materials to irradiation by ion beams, or neutrons can also drive the system in a complex configuration. Sometimes the system is so perturbed that order-disorder phase transitions driven by irradiation occur in alloys. Phase transitions induced by irradiation can also be observed in simple oxides like zirconia where the solid transforms from one crystallographic structure to another. Irradiation-induced transitions have also been observed in more complex oxides. Mechanisms leading to such phase transitions under irradiation are not yet understood.
- Thermodynamic quantities are central to the assessment of the stability and/or the chemical reactivity of solid phases. These quantities have not all been established, whether upon experimental or theoretical grounds.
- Not only materials constraints (e.g. fatigue, corrosion, thermal creep, etc.) are central but also the interplay of all coupled systems, activated by a combination of the different forms of constraint; addressing this requires interdisciplinary research.

In such a context R&D is indispensable. Joint and comparative studies are most effective in supporting the development of various categories of innovative fuels (including clad materials). Interdisciplinary joint studies are useful in gaining multi-scale understanding of fuels and structural material for nuclear systems and in dealing with the scientific and engineering aspects of nuclear materials. In particular, they aim at establishing multi-scale models and simulations as validated predictive tools for the design of nuclear systems, fuel fabrication and performance. Collaborative R&D is a powerful tool to promote the exchange of information on models and simulations of nuclear materials, theoretical and computational methods, experimental validation and related topics. Up-to-date information, data, models and expertise are all shared. Combining experimental and theoretical knowledge from diverse fields of research can benefit each.

Research effort

Many bottlenecks still exist and call for particular research effort. Two examples will illustrate the specific and generic problems raised by nuclear materials. The example of developing numeric models highlights the important contribution to materials sciences of nuclear R&D, centred as it is on radiation phenomena, their modes of action and their impact on the utilisation properties of materials. The second example illustrates not only the specific features but also the general nature of the problems to be solved regarding lifecycle thermodynamic properties of materials.

The experimental study of irradiation effects in materials is very expensive because it requires rare, dedicated infrastructure (experimental nuclear plants, hot laboratories). Significant effort thus has been devoted to developing numeric tools to model irradiation effects in nuclear materials. To reduce the time and resources needed to develop new fuels and structural materials, researchers have concentrated on identifying fundamental problems amenable to analysis by modelling/simulation



and experiments. Modelling is typically used to describe the thermodynamics of point defects and the irradiation-induced phase. A major goal is to build a coherent set of tools operational for any physical model addressing multi-scale materials. Such a platform may include, but is not limited to the following:

- atomistically informed modelling and simulation of nuclear fuels and structural materials at progressively greater scales of time and size, with due attention to radiation damage effects and to the methodologies needed to achieve inter-scale integration;
- validation of simulations and model predictions by benchmarking exercises and identification of experimental data that would be most critical to this validation;
- creating and maintaining synergy of experimental and testing practices; establishment of reference experimental and simulation datasets and databases, aiming at improving the joint utilisation of modelling/simulation and experimental techniques;
- development of new applied mathematics and software tools such as new data storage and algorithmic methods, particularly those of common interest for fuels and structural materials;
- integration of results from multi-scale modelling and simulation into performance codes and materials qualification processes, as well as into multi-physics environments, such as the coupling of changes in materials' properties and neutronics.

For practical applications, the determination of accurate diagrams describing the equilibrium state of multi-component materials is an important issue. Specialised software is definitely of great use for both calculating acceptable diagrams and giving access to a complete thermodynamic database. Inputs (selected structures and values) must be chosen with care, and the critical analysis of the output results also presents challenges. Unfortunately, because of the above-mentioned difficulties quality-assured quantities are seldom available. Furthermore, the more severe operating conditions foreseen in Generation IV nuclear vessels create an even more stringent demand for thermodynamic data of quality. A detailed assessment of the thermodynamic quantities of all phases of the complex fuel systems is needed in order to predict the behaviour of materials (chemical compatibility for instance) in the temperature range of of 1000-2000°C. Such detailed assessment also aides the definition of the practical conditions for fuel material processing.

Fission products and minor actinide elements must also be taken into account to predict the physicochemical behaviour of irradiated fuels under both normal and accidental conditions. For severe accident conditions, a thermodynamic database constitutes a useful tool for interpreting future experiments on fission product release. It also allows prediction of the temperature at which liquid formation takes place. Databases on nuclear materials must contain all possible compositions of solid solutions and not only simple compounds.

Vast range of applications

The knowledge acquired and methods developed during nuclear materials investigations have a vast range of potential applications beyond the specific conditions of the nuclear domain. A great many physical phenomena and basic mechanisms which intervene in the nuclear field are just as pertinent in regard to the behaviour of these materials under less severe conditions, as well as in completely different utilisations and environments. ■