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Review

Materials for Sustainable Nuclear Energy: A European Strategic Research and Innovation Agenda for All Reactor Generations

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Abstract: Nuclear energy is presently the single major low-carbon electricity source in Europe and is overall expected to maintain (perhaps eventually even increase) its current installed power from now to 2045. Long-term operation (LTO) is a reality in essentially all nuclear European countries, even when planning to phase out. New builds are planned. Moreover, several European countries, including non-nuclear or phasing out ones, have interests in next generation nuclear systems. In this framework, materials and material science play a crucial role towards safer, more efficient, more economical and overall more sustainable nuclear energy. This paper proposes a research agenda that combines modern digital technologies with materials science practices to pursue a change of paradigm that promotes innovation, equally serving the different nuclear energy interests and positions throughout Europe. This paper chooses to overview structural and fuel materials used in current generation reactors, as well as their wider spectrum for next generation reactors, summarising the relevant issues. Next, it describes the materials science approaches that are common to any nuclear materials (including classes that are not addressed here, such as concrete, polymers and functional materials), identifying for each of them a research agenda goal. It is concluded that among these goals are the development of structured materials qualification test-beds and materials acceleration platforms (MAPs) for materials that operate under harsh conditions. Another goal is the development of multi-parameter-based approaches for materials health monitoring based on different non-destructive examination and testing (NDE&T) techniques. Hybrid models that suitably combine physics-based and data-driven approaches for materials behaviour prediction can valuably support these developments, together with the creation and population of a centralised, "smart" database for nuclear materials.

Keywords: nuclear materials; nuclear materials science approaches; digital techniques; strategic research agenda

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1. Introduction

1.1. Towards Sustainable Nuclear Energy

With 685 TWh_e produced in 2020, which corresponds to ¼ of the total production from all sources, nuclear energy is the single largest source of low-carbon electricity in the European Union; see Figure 1 [1]. Thus, nuclear energy is playing an important role, in alliance with all renewables, towards climate-neutrality in Europe by 2050. Despite widespread perception that nuclear energy is being abandoned in this continent, due to the undeniable decline in the last 20–15 years and especially after the Fukushima accident, an analysis of the national energy and climate plans (NECP) and other official sources [2–4] reveals that, by 2045, the number of operating reactors in Europe will probably be only between 5% and 12% less than now, with almost unaffected total installed power capacity [5]. Recent decisions of some countries suggest that it may even eventually increase in the medium-to-long term. This will happen via long-term operation (LTO), i.e., pro-active extension of the lifetime of reactors, as well as power uprates of operating reactors and new builds. As a matter of fact, while some countries are progressively phasing out, others will keep using nuclear power, or even expand their fleet. The likely European Union (EU) decision to include nuclear energy in the taxonomy for sustainable finance will probably facilitate and perhaps amplify this process. LTO is indeed recommended by the International Energy Agency (IEA) as an important affordable contributor to progressive electricity decarbonisation and in the EU the economic case for nuclear lifetime extension is especially strong, even if the decrease in wind and solar photovoltaic costs accelerates [6]. Accordingly, LTO is a reality in essentially all nuclear European countries, even some of those that are eventually planning to phase out [5]. In addition, several European countries, including non-nuclear ones, or countries that are planning to phase out, have research and development interests in next generation nuclear systems, of the kind described further on. In this framework, it is here put forward that the concerned research community in Europe needs to be at the forefront and ready to support with effective and cutting-edge strategic agendas the continental nuclear developments, in order to guarantee ever increasing sustainability.

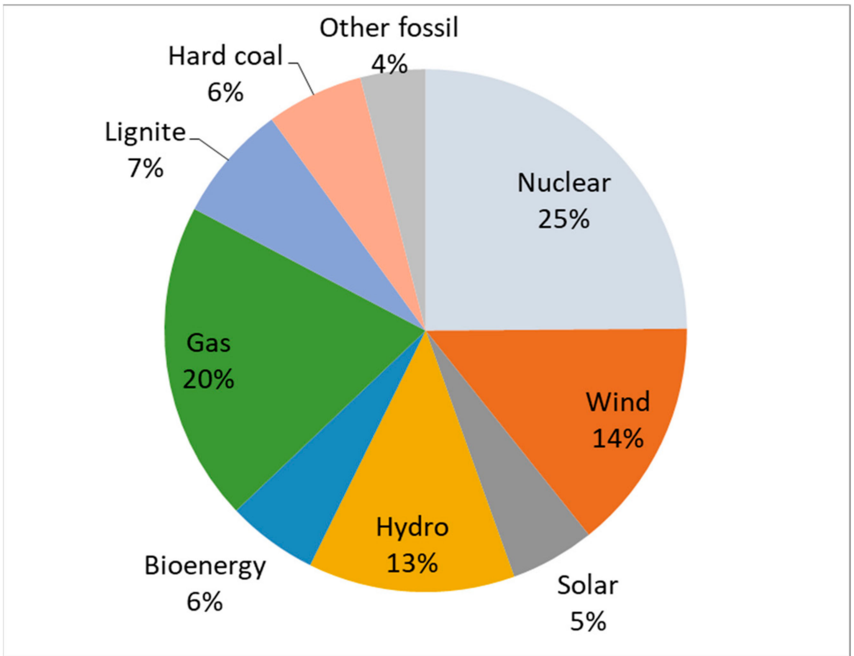

Figure 1. Electricity generation by fuel in the European Union in 2020 [1]. The sum of renewables (wind, solar and hydro) exceeds the contribution of nuclear, which, however, represents the single major low-carbon electricity source.

Five concerns regarding nuclear energy are widespread in the public opinion, and often also among the decision-makers, of several European countries and hamper the full-hearted use of nuclear as a sustainable part of the energy transition. They therefore need to be seriously addressed. These are: safety of operation and severe accident risk; management of long-lived nuclear waste; economics (especially for initial investments and back-end costs) and long construction times; limitation of fuel resources; and possible misuse of fissile materials.

In the short term, these issues need to be addressed with current light water-cooled reactors (LWR) of second or third generation (GenII/III) and the Gen III+ new builds. There are indeed still ample margins, through research and development, to increase substantially the safety, performance, economy and sustainability of nuclear reactors of established technology, as well as to further reduce their already low impact on the environment. Continuous improvements of operational practices and nuclear safety of current reactors, in the context of an increased flexibility of the network, are routinely pursued by the European nuclear industry and are already the object of extensive research in Europe and elsewhere [7–10]. Deep geological disposal of highly radioactive waste is on the other hand recognised as a safe and secure long-term solution by most nuclear countries [11,12], even though some wish to postpone its implementation and evaluate other options [12]. Finally, small and medium-size modular reactors (SMR) that use light water as coolant and moderator are at reach of known technology and may be a relatively short-term answer to the high capital costs and long construction times that currently hamper new nuclear builds, especially in Europe, while offering better flexibility and adaptability to different uses, in co-habitation and collaboration with intermittent renewables [13,14]. SMRs feature a power output between 10 (or less) and 300 MW_e and a construction based on the idea of higher degrees of modularisation, simplification and standardisation compared to larger nuclear reactors [13]. A sub-class of them is denoted as micro-reactors: these would produce 1–20 MW_e and would be fully factory fabricated, transportable and self-adjusting [13–15]. SMRs are largely perceived as game-changers by the nuclear industry, provided that national legislations accompany and facilitate standardised modular construction needs in terms of regulations, while global deployment will require a certain degree of harmonised licensing [13]. Three water-cooled SMRs are being designed in Europe [16–18]. Water-cooled SMRs may also be used for combined electricity and heat generation, thus expanding the uses of nuclear energy to applications such as hydrogen production via high temperature steam electrolysis [19,20], sea water desalination (largely already a reality) [21] and district heating [17,22,23].

In the longer term, the above nuclear energy issues can be dealt with, and the overall sustainability greatly increased, through the commissioning and deployment of fourth generation (Gen IV), liquid metal or molten salt cooled, fast neutron reactors, along with the facilities that are needed to close the nuclear fuel cycle [24]. By pushing the burnup to high values, i.e., letting the fuel remain for longer in the reactor to extract more energy, fast reactors can produce more ^{239}Pu from the ^{238}U by neutron capture than fissile nuclei consumed by fission [25]. Fast neutron systems thus enable circular economy: through recycling, they significantly improve the utilization of natural resources, strongly reducing the need of mining and ensuring fuel availability and self-sufficiency for centuries and perhaps millennia. Different fuel designs and appropriate reprocessing strategies can furthermore make the diversion of fissile materials more difficult [26,27]. Another virtue of these systems is that, since Pu is eventually removed from the fuel for reuse, they enable the long term radiotoxic impact of waste to be abated. This is especially true when minor actinides (heavy elements present in low quantity, but significantly contributing to long term radiotoxicity and heat production) are transmuted in the reactor itself into shorter lived fission products, after sufficiently high burnup [28], or using dedicated devices such as accelerator driven systems [28,29]. These practices can reduce the volume of remaining radioactive waste and the emitted heat flux by one order of magnitude, and the radiotoxicity timespan to a few hundred years [28], thereby significantly relieving the requirements of anyway necessary geological disposals. Moreover, GenIV reactors will feature high safety standards because the use of liquid metals (generally either sodium or lead alloys) or molten salts as coolants enables operation at atmospheric pressure and facilitates the design of passive systems [30]. Fast reactors must indeed use non-aqueous coolants, because moderation (neutron slowdown) is not sought for [25]. This obliges to operation at temperatures well-above those of current LWR (about 300 °C), because liquid metals or molten salts need to remain fluid and must thus be kept above their melting point, in ranges between 400 and 500 °C as inlet temperature. With these fluids it is thus envisaged that outlet temperatures up to 700 °C or above should be reached, thereby increasing significantly the thermal efficiency with respect to current LWRs. In summary, GenIV systems significantly reduce the quantity of the transuranic waste and its long-term hazard, optimise the use of fuel resources available on earth and enable high safety standards. They are thus expected to be attractive for the public opinion at large, as a fully sustainable low-carbon source of energy. Some experience on these reactors exists already (see Table 1). Sodium-cooled fast reactors have been operated in Europe [31] and are still operated outside [32], while a lead-cooled fast reactor demonstrator is being constructed in Russia [33]. However, for a number of reasons that span from technological to economic and political, no widespread commercial deployment of GenIV systems seems likely until beyond the mid of this century, at least not in Europe. GenIV reactors, therefore, will hardly contribute to the decarbonisation of society and economy by 2050. Nor will fusion, which, by targeting for 2050 the demonstration of the connection to the grid for the first time [34], is unlikely to be commercially viable and deployed before the end of the present century. Annex 1 describes the GenIV prototypes that are being designed in Europe.

Gas-cooled reactors target high operation temperature and are somehow a bridge between current and future nuclear generation. Graphite moderated power reactors cooled with CO_2 exist and are still operated in the UK. They reach outlet temperatures in excess of 600 °C [35]. High temperature reactors (HTR) that also used graphite as moderator, but adopted different fuel designs and employed He as coolant, have been operated in the past, with outlet temperatures round 750 °C [36–38]. They are thus known technology and can therefore be already considered for low-carbon industrial heat production in addition to electricity (cogeneration), including hydrogen production by thermal, rather than electrolytical, processes, provided that they are considered attractive enough by industrial heat and hydrogen consumers. Importantly, the SMR concept can be extended to any nuclear technology, leading to the design of *advanced* modular reactors (AMRs) that use non-aqueous coolants. Therefore, small and modular graphite moderated, gas-cooled HTRs that operate above 600 °C appear as an especially attractive technology that is already at reach to flexibly provide carbon-free industrial or district heat [13,14,21,39]. One has recently started to be operated in China [40]. High safety levels are guaranteed by the combination of the high thermal stability of graphite with the reduced power of the system, which should indeed enable significant reduction of the Emergency Planning Zone [41], and ideally its removal. In a somewhat longer term, liquid metal or molten salt cooled AMR also appear to be attractive solutions [13,14,42]. In addition, the GenIV portfolio foresees two so far never built gas-cooled concepts: the very high temperature reactor (VHTR) [43] and the gas-cooled fast reactor (GFR) [44]. Both target temperatures in excess of 800 °C, possibly even in excess of 1000 °C. They could both provide heat for a wide variety of industrial applications, in addition to producing electricity with very high efficiency, on the order of current combined-cycle fossil gas plants (~50%–60%). The GFR would additionally include the benefits of waste reduction and optimal use of resources of fast systems, such as those described above. Yet, they are both considered very long-term developments. Finally, another GenIV concept that is often considered as an evolution of LWR, and thus in principle more readily available, is the super-critical water-cooled reactor (SCWR) [45]. Table 1 summarises the main features of GenIV technology concepts and illustrates the existing experience. Annex 1 includes some information on related design work in Europe.

In this planned journey towards safer, more efficient, more economical and overall more sustainable nuclear energy, materials and material science, thus research on materials, play a crucial role. This is discussed in the next section.

Table 1. Main features of next generation nuclear systems and existing experience, following GenIV-related nomenclature and references [43–47].

System Abbreviation	Coolant	Neutron Spectrum	Reactor Type Already Built	Power Reactors in Operation
SFR	Liquid sodium	Fast	Yes [31,32]	Yes [32]
LFR	Liquid lead	Fast	No [1]	No
GFR	Gas (He or other)	Fast	No	No
SCWR	Super-critical water	Thermal or Fast	No	No
MSR	Molten salt	Thermal or Fast	Yes [46]	No
HTR	Gas (He or other)	Thermal	Yes [36–38]	Yes [40]
VHTR	Gas (He or other)	Thermal	No	No
ADS	Lead-bismuth eutectic	Fast	No [1]	No
Fusion	Water/He/Pb-Li/ . . .	(Very) fast	No	No

[1] PbBi was used as coolant in submarine fast reactors [47]. LFR is under construction in Russia [33].

1.2. Role of Materials and Materials Science for Sustainable Nuclear Energy

One of the main reasons why not all GenIV systems are technologically ready, yet, and that determines the shorter- or longer-term deployment of these systems, is the fact that the targeted high temperatures, combined with very high neutron dose in core components (due to the high burnup) and with the use of non-aqueous coolants, will subject materials and components to especially degrading conditions. Currently, no material of industrial production can sustain the target GenIV operating conditions for sufficiently long time to provide the reliability and availability that is required from crucial components, so as to ensure economical commercial viability of systems of this type. Thus, the availability of materials with superior resistance to irradiation and corrosion in a wide enough temperature window is an essential point to make GenIV reactors a reality [48]. The realization of thermonuclear fusion on earth largely shares similar, if amplified, challenges [34,49,50]. In all cases, demonstrators targeting less ambitious operating conditions need to be built, proceeding by stages that include materials and component progressive qualification for increasingly demanding conditions, before commercial plants can be designed (see Annex 1). Thus, the availability of a large palette of materials for various objectives, with superior resistance to irradiation and corrosion in a wide enough temperature window, is crucial to make nuclear energy fully sustainable.

Concerning current generation reactors, lifetime extension can be (and indeed has been) granted with current materials technology, while light water-cooled or high-temperature gas-cooled SMRs can be designed by making use of known materials. However, innovative materials solutions that, starting from established references, enable safety and efficiency to be increased, or costs to be abated, with equal or improved efficiency and safety, or that importantly ensure that the component supply chain can be efficiently maintained or improved, are an asset for current generation nuclear energy, as well. These importantly include the use of advanced manufacturing techniques. Tools that are capable of better predicting the behaviour of materials and components in operation and in accidental scenarios are an obvious support to increased safety. In addition, aspects of circularity and life cycle assessment necessarily require specific attention in connection with sustainable decarbonisation using nuclear. These range from a closer attention to the supply of raw minerals, to the optimization of component lifetime by appropriate maintenance and replacement, via monitoring of materials' and components' health in operation, and to recyclability or (if possible) reusability, thus anticipating decommissioning issues. These are all issues to be addressed with the tools of materials science. Thus materials science is crucial to increase the sustainability of nuclear systems of any generation and type.

In 2019 the Joint Programme on Nuclear Materials of the European Energy Research Alliance (EERA JPNM)—see Annex 2—produced a Strategic Research Agenda to ensure that suitable structural and fuel materials are available for the design, licensing, construction and safe long-term operation of GenIV nuclear systems [51]. In parallel, the Sustainable Nuclear Energy Technology Platform (SNETP) and its three pillars—see Annex 2—updated their Strategic Research and Innovation Agenda, addressing the whole spectrum of nuclear reactor generations, including considerations on materials of specific relevance for current generation reactors [52]. In 2021 a more structured discussion was launched concerning the need to organise the European nuclear materials research community into a better structured collaboration framework, with a single vision through reactor generations, as part of the ORIENT-NM project [53]. This paper summarises the salient points that emerged from these documents and discussions concerning nuclear materials in Europe, exemplified by structural and fuel materials. As a result, we propose a research agenda that, based on the exploitation of modern digital technologies combined to materials science practices, pursues a change of paradigm, which is deemed suitable to promote innovation and should be the way to go for the future in the nuclear materials field, in Europe and elsewhere. The structure of the paper is as follows: Section 2 overviews the type of structural and fuel materials that are used in current generation reactors, and the wider spectrum of those that are likely to be used in next generation ones, summarizing the relevant issues; Section 3 describes the materials science approaches that are common to all nuclear materials, identifying for each of them what the goal of a research agenda should be; these goals are finally discussed in Section 4 in terms of opportunity and feasibility, leading to the conclusion in Section 5.

2. Materials for Current and Future Nuclear Systems

2.1. Structural and Fuel Materials for Current Generation Reactors and Relevant Issues

LWRs, which are water-cooled and also water-moderated, represent more than 80% of the operating nuclear power plants (NPP) worldwide (GenII/III). The most common reactor design is the pressurised water reactor (PWR, about 80% of the LWRs), followed by the boiling water reactor (BWR, 20%). Heavy-water cooled and moderated reactors (e.g., CANDU, CANadian Deuterium Uranium) are the only other design that represents a non-negligible fraction of the global share of operating NPPs (about 11% of the total). The remaining ones are graphite moderated, either gas-cooled or water-cooled reactors. All of these types exist (or existed at some point in time) in Europe (EU and associated countries). The trend in new builds is towards almost exclusively PWRs (GenIII+).

The main pressure boundary components in LWRs, i.e., the reactor pressure vessel (RPV), the pressuriser, and the steam generator shells, as well as the turbine (except the blades) and the condenser, are generally made of low-carbon, low alloy ferritic (bainitic) steels. The secondary circuit piping in PWR is also made from steels of this type. Austenitic stainless steels, particularly AISI 304 and/or 316L in P/BWR, and Ti-stabilised (similar to AISI 321) in the Russian PWRs (VVER), dominate as core structural materials, as well as for the primary circuit and its components. Steam generator tubes are often made of Ni-based alloys. Austenitic stainless steels and Ni-based alloys are selected because of their good resistance to water corrosion up to high temperature. Thus, austenitic steels (AISI 308 or 309) are also used as liners on the inside surface of pressurised vessels for corrosion protection. Low-carbon, low alloy steels have, in turn, the advantage of superior weldability through thick sections and 4–5 times lower price than austenitic steels. Both are important items for large components such as the pressure vessel. Fuel pin cladding in all current LWRs are made of Zr alloys, which exhibit very low neutron absorption cross section. In the case of heavy-water reactors of CANDU design, low-neutron absorbing Zr alloys are used also for the pressure tubes that contain each fuel assembly, allowing the use of natural uranium as fuel. Because of industrial constraints and safety requirements all these materials are unlikely to be changed: it is indeed recommended that these components are manufactured with well known, easy to use materials, the properties of which are vastly known from many years of experience [54]. Cautious changes are however possible for new builds, in terms of minor compositional and heat treatment tuning, within specifications, as well as the introduction of more restrictive specifications [54]: they are part of the continuous improvement that, in the past, led to changes of composition for materials of a specific components, based on field experience. With a view to continuously increasing safety, in the case of these materials and components what matters most is: (1) to be able to predict increasingly better their behaviour in operation, in order to estimate correctly their residual life, optimise inspection plans and foresee timely repairs and replacements, thereby guaranteeing that all components and systems maintain their integrity and functionality at all times and in all circumstances; (2) especially in a framework of LTO, to be able to optimally replace and repair components, making sure that this is done in full compliance with nuclear safety regulations. The former requirement essentially calls for continuously improved models, based on physics as well as on experience, and automatised material health monitoring strategies; the latter requires that the supply of materials and components according to nuclear specifications is guaranteed over decades in a timely and affordable way. These issues are discussed in a broader framework in Section 2.4.

Concerning fuels and fuel elements, these must: (1) Provide the power expected during their whole stay in reactor; (2) Use the fissile elements as best as possible to reduce the cost of energy production; (3) Confine the fission products inside the fuel elements in all operating and accidental conditions; (4) Maintain dimensional stability within design margins. All LWRs around the world currently use ceramic uranium dioxide (UO_2) as fuel, encased in the Zr-based alloy cladding. In most cases the uranium is enriched to 3–5% ^{235}U. Some reactors use mixed U-Pu oxide (MOX) fuels. The oxide fuel/Zr-alloy system has been optimised over many decades and performs very well under normal operation and anticipated transients. However, because of the highly exothermic nature of the chemical reaction between Zr and steam, in case of temporary loss of core cooling with uncoverage of part of it, the resulting excess generation of heat and hydrogen may produce significant undesirable core damage. This happened in the events that followed the Fukushima Daiichi power plant accident, caused by combined earthquake and tsunami in 2011. Because of this, global interest has expanded in the last ten years to explore fuels with enhanced performance during such rare events, the so-called accident-tolerant fuel (ATF), which involves both the fuel itself and, especially, the cladding [55,56]. Both should exhibit higher thermo-mechanical stability and be designed and qualified to remain intact for a sufficiently long time even when subject to accident conditions. Such type of fuel, in combination with other systems, is expected to provide sufficient time for intervention in case of accident, avoiding too severe outcomes, while offering additional benefits in case of more frequent off-normal situations, as well as normal operation [57]. The possible ATF cladding materials, all of them still necessitating qualification, range from suitably coated Zr alloys (the simplest solution from an industrial point of view), to advanced ferritic/martensitic (F/M) steels with improved creep resistance, or refractory metals, like Mo, or SiC fibers in bulk SiC (SiC_f/SiC) composites. Interestingly, except for coated Zr alloys, all ATF cladding materials are also considered as structural materials for next generation reactors (see next section). On the fuel side, research on enhanced performance has focused on improved UO_2 (doped with oxides such as Cr_2O_3, Al_2O_3 or SiO_2, or with high-thermal-conductivity metallic or ceramic phases, in order to enhance the fission gas release process by increasing the grain size and optimise mechanical properties), higher density fuels (nitrides, carbides, silicides and metals), or microencapsulated fuels (TRISO-SiC composites) [57,58]. The last ones are intrinsically accident tolerant and have been already used in HTR that were operated in the past; the challenge is to develop similar accident tolerance for LWRs

It should be noted that important materials for current generation reactors, which are also the focus of research, are concrete for the contention building and polymers for cables and tubes. Also important are functional materials such as for sensors or for neutron control. These, however, are not addressed in this paper.

2.2. Structural Materials for Next Generation Nuclear Systems and Relevant Issues

GenIV liquid-metal cooled reactor demonstrators are expected to operate between ~400–550 °C, with off-normal excursions up to 600 °C [51]. However, the target for commercial plants is an outlet temperature in the 600–700 °C range, or even beyond [51,59,60]. Molten-salt cooled systems need to shift the inlet temperature above 500 °C to keep the coolant fluid and also target 700 °C or higher outlet temperatures in commercial plants [51,59,60], while gas-cooled systems target 850 °C or beyond [51,61]. In the latter, temperatures around 2200 °C may be reached at the centre of the fuel in normal conditions, while temperatures may exceed 1000 °C in structural materials in off-normal conditions. These temperatures, coupled to temperature gradients up to, in extreme cases, 500–1000 °C/mm [62], will inflict severe thermal and mechanical stresses on the fuel and plant components, requiring materials with high thermal stability and resistance to cyclic loading. Cooling fluids are, in addition, chemically hostile environments, with detrimental effects on structural materials in terms of corrosion, dissolution, or erosion [63–70]. All of these processes lead to thickness reduction, which can be strongly penalizing, especially for thin components such as cladding. In addition, all of these coolant effects are exacerbated by high temperature, to the point that they are often the main limiting factor for the outlet temperature. Inside the fuel pin, finally, chemical interactions between cladding materials and fission products may be a concern [71], as well. On top of this, core materials are exposed to varying levels of irradiation dose and dose rates: 1 dpa/day in the fuel [72], 100 dpa or beyond in the cladding over its time of irradiation [73], but likely less than 5 dpa in the in-vessel structures over the whole reactor lifetime [74] (Dpa, displacements per atom, are the unit used to measure the radiation dose received by materials, irrespective of spectrum and type of impinging particle [49,75]). Figure 2 illustrates the operating regimes envisaged for GenIV prototypes/demonstrators in Europe, including possible commercial plant target conditions, as compared to current generation LWRs.

Exposure to irradiation is known to produce a number of detrimental consequences on materials. In structural materials these range from hardening and embrittlement with loss of elongation to changes of dimension and shape due to swelling and creep [76–81]. In addition, if the neutron spectrum leads to transmutation with production of helium (α particles) and hydrogen(protons), depending also on material composition, the mentioned effects may be significantly exacerbated and the temperature ranges of susceptibility increased on the high side, this problem being especially serious for fusion and Ni-containing materials [77–81]. Radiation-induced hardening with subsequent loss of elongation and embrittlement typically occurs when irradiating at low temperature, where "low" depends on the material [77,79,82], for instance in steels the threshold is roughly below 400 °C, but in tungsten alloys it is below 800 °C [82]. Hardrning and subsequent embrittlement appear to some extent from the very beginning of the irradiation and increase with dose, but generally saturate at high enough dose [77,79]. In contrast, dimensional changes occur only at high enough dose, on the order of tens of dpa [77–81]: they do not necessarily saturate with increasing irradiation (only the rate does) and typically they only appear above a certain irradiation temperature (about 400 °C in steels) [77,83]. Clearly, these high temperature/high dose effects, which are hardly observed in current generation reactors, are expected to be significant in next generation ones.

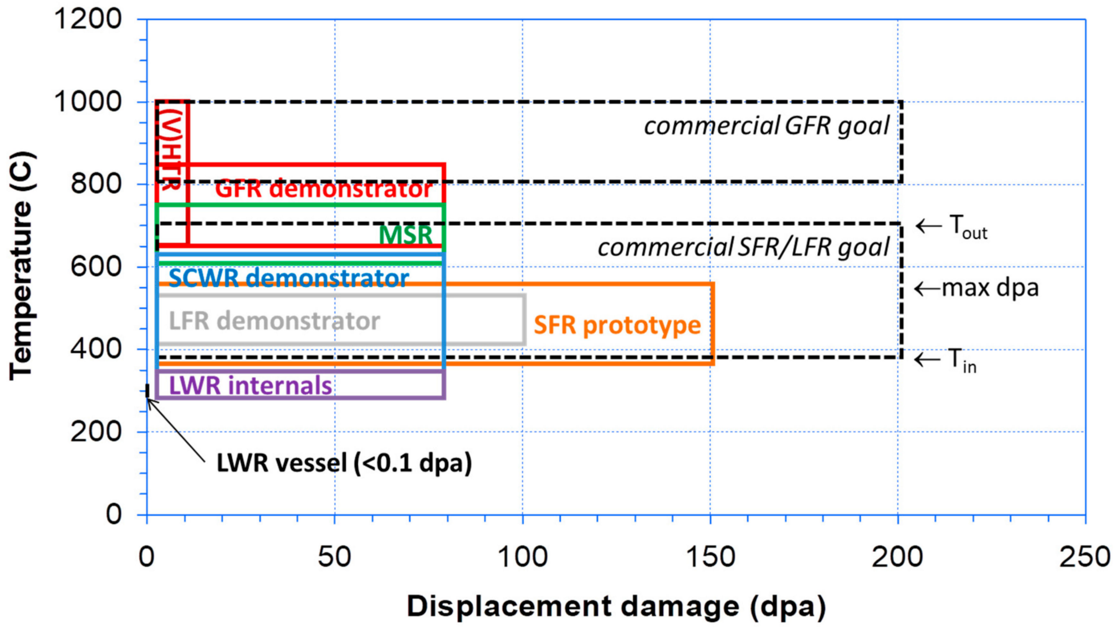

Figure 2. Schematic and indicative illustration of the operating conditions envisaged in European designs of GenIV prototypes/demonstrators, as compared to current LWRs (assuming 60 years of operation) and commercial GenIV reactors. The temperature range is defined by inlet/outlet temperatures. The maximum dpa concerns structural components. (Cf. Table 1 for abbreviations).

Only a few classes of materials have the potential to sustain the above described operating conditions for the required operation time, depending on the function of the corresponding component and the type of system [84]. These classes of materials are wide, because no final choice has been made, yet, and because the variety of next generation nuclear systems is significant. They only partially overlap with the materials that are being used in current LWR, namely low alloy steels for the vessel, austenitic steels for internals, and zirconium alloys for the cladding (see previous section), as is made explicit in Table 2. Yet, some of these materials are also considered for ATF cladding [56]. They are briefly overviewed in what follows.

The GenIV demonstrators and prototypes planned in Europe (Annex 1) [85,86], and not only in Europe [87], envisage the use of austenitic steels as the dominant class of in-core structural materials, almost irrespectively of the type of coolant. Particularly, 316L(N) is considered for most components, in most systems, including the vessel, while 15-15 Ti (also denoted as D9 or 1.4970) is the choice for the cladding and other fuel element parts in essentially all designs. The reason is that these materials are a good compromise between several requirements. However, with these materials no design solution will ever enable the conditions that are targeted for highest efficiency and best economy in commercial GenIV plants to be reached. Thus, prototypes and demonstrators will have to work at temperature and irradiation dose regimes that may be significantly less ambitious than those targeted in commercial plants (Figure 2). However, the existing return of experience from use of these austenitic steels in fast reactors that were built and operated in the past, such as, e.g., Phénix and Superphénix in France [31], provides a wealth of experimental data. On these bases, design rules have been already established for them and introduced in standard codes: this is crucial for executive design and timely licensing. Once the demonstrator is in place, it can be used as a laboratory for further materials upgrade, through qualification in environment. A staged approach is thus generally adopted by designers, with a start at temperature and irradiation levels compatible with currently available materials, to be increased in later stages. Research on materials can thus be split into a number of steps, thereby enabling a distinction between near term and long term application.

Table 2. Summary of classes of structural materials through reactor generations. RPV = reactor pressure vessel, F/M = ferritic/martensitic, ATF = accident tolerant fuel, ODS = oxide dispersion strengthened, AGR = advanced gas reactor, (V)HTR = (very) high temperature reactor, GFR = gas-cooled fast reactor, HEA = high entropy alloys, CCA = compositionally complex alloys.

Class of Materials	Use in GenII/III	Use in GenIV	Notes
Low alloy bainitic steels	Pressure vessel, pressuriser, steam generator shell, turbine, condenser	None	Upper limit of operation temperature window <400 °C
Austenitic steels	Core components (except cladding), liner RPV	Vessel, core components including cladding	Experience from use in thermal and also fast reactors. Improved swelling resistance (e.g., Ti stabilization) and corrosion protection in heavy liquid metals (e.g., coatings or Al-containing alloys) needed—see Annex 3.
Zr alloys	Cladding, power channels in heavy-water reactors	None	Historical example of material development specific for nuclear [54]
F/M steels	None (but improved versions considered for ATF cladding)	Cladding and core components where swelling must be low	Swelling-resistant, good thermal physical properties. Creep (e.g., ODS), and corrosion resistance (e.g., coatings or Al-containing alloys) need improvement—see Annex 3.
Ni-base alloys	Steam generator tubes	Steam generators, in the longer term core components for high temperature operation	Good corrosion and temperature resistance. Susceptible to embrittlement due to He and H production via transmutation when irradiated: improvement needed (e.g., ODS)—see Annex 3.
Refractory alloys	None (but some are considered for ATF cladding)	In-core and out-of-core components (also vessels) where operation temperatures round 800 °C are expected	Wide spectrum of possibilities: Ni-base and Ti-base alloys may enter this category, composed by Mo-, Nb-, Ta- and V-alloys (W-alloys for fusion)—see Annex 3.
Graphite	Still used as moderator only in the core of UK AGR	Moderator with structural functions as well in (V)HTR concepts	Vast experience on its use. Very high thermal stability. Since it is a moderator, its use is limited to thermal spectrum reactors—see Annex 3.
Ceramic materials (SiC_f/SiC, other)	None (but SiC_f/SiC considered for ATF cladding)	Cladding and core components in VHTR and GFR	Composites and other ceramics have been long studied, but are still far from being fully qualified and codified. Design rules need to account for brittleness. Often costly—see Annex 3.
Prospective materials (HEA/CCA, Max phases, . . .)	None (but speculation of use for ATF cladding)	Mainly cladding and coatings, but not clearly identified	These materials are investigated because of their promising properties, but even more because of the possibility of applying modern materials development techniques based on combinatorial fabrication—see Annex 3.

Depending on the system, other known materials may also enter demonstrator and prototype designs, e.g., ferritic/martensitic (F/M) steels [79,88] and, for higher temperatures, Ni-base alloys [89,90] or graphite [91]. However, in demonstrators and prototypes these two metallic materials are mainly considered for out-of-core components [92], such as steam generators. In contrast, graphite is considered for HTR cores, thanks to the significant experience that exists already on its use [91]. There are reasons to consider F/M steels and Ni-base alloys also for core components, particularly for systems cooled with liquid metals or molten salts. But this will likely happen only in second phases of demonstrators or in perspective commercial reactors, provided that these materials, or more likely improved versions of them, are previously qualified for the relevant operating conditions and codified for design. For instance, F/M steels exhibit better thermal properties and only swell above 200 dpa [79,88], which is crucial to attain high burnup, but they suffer from other limitations that need to be relieved, e.g., low temperature embrittlement and unsatisfactory creep resistance [79,88]. The latter calls for improvements, e.g., by introducing oxide dispersion strengthening (ODS) against creep [93], which has been long studied, but is not yet sufficiently developed for component design and operation. As a perhaps shorter-term alternative, pathways to improve the swelling resistance of austenitic steels do exist [94]. More details, including aspects of corrosion protection, are provided in Annex 3.

Systems that target operation around or beyond 800 °C can only be conceived using, as structural materials, either Ni-based superalloys [90], such as alloy 800 [95], or, more appropriately, refractory metallic alloys [90,96,97]. Higher temperatures are the realm of ceramic materials: in addition to graphite, the base core material for the VHTR, also SiC/SiC composites [98–100], which are main target material for GFR core components, as well as a plethora of other possibilities, depending on component and function [90]. However, these materials are generally not fully defined: especially for refractory alloys, innumerable possibilities and combinations exist [90]. They are therefore far from being qualified and codified for design under the target conditions. In such a long term perspective, further gateways to improved future reactor performance are opened considering other perspective materials [101], e.g., ODS-Mo alloys [102], high entropy alloys (HEA) [103], better called compositionally complex alloys (CCA) [104], or MAX phases [105]. The spectrum of possibilities is very wide and it may be difficult to orientate in it.

Table 2 summarises the classes of structural materials for nuclear applications through reactor generations.

2.3. Fuel Materials for Next Generation Nuclear Systems

Nuclear fuels and fuel elements for next generation reactors may differ widely, depending on the reactor concept, in geometrical configuration, composition, cladding and even physical state. Reactor fuels are based on compounds of one or more fissile and/or fertile nuclides, mainly of U and Pu. They can be either refractory oxides, typically U oxides and MOX, which are also used in current generation reactors [106–109], or other ceramics, such as carbides [110], nitrides [111,112] and silicides [107,113,114], as well as metallic alloys [115]. Other fuel concepts consider ceramic/ceramic or ceramic/metal composites [116], as well as fluid molten salt fuels [117]. Solid fuel may appear in various geometries: rods, plates or pellets. U oxides and MOX are the most industrially used fuel materials [107]. MOX is indeed currently the reference fuel for most fast neutron reactor demonstrators and prototypes in Europe, mainly because this class of fuels was used in the European fast reactor programme that led to the construction of Phénix and Superphénix [118]. The licensing of future fast reactors systems can thus take advantage of the extensive knowledge base on MOX fuel. The fabrication method has a large influence on the fuel performance, since it determines essential properties such as the porosity, the size of the Pu-rich agglomerates and the impurity levels [108,109,118,119]. Furthermore, reactor core designs have evolved, so different pellet geometries are considered, e.g., high-density pellets with an annulus to regulate centre-line temperatures or low-density full pellets [108,118]. Finally, reactor cores also differ because of the differing coolants and may be operated at various temperatures and power ratings [120], thus they necessitate further specific investigations. ADS, in addition, bring distinct issues that may impact fuel performance, for example the thermal stresses induced by frequent proton beam trips [121,122].

The sustainability of the fuel cycle can be significantly increased by Pu multi-recycling. This will, however, affect the Pu concentration and its isotopic vector in the fuel and lead to higher Am contents (from ^{241}Pu), which will increase the radioprotection requirements during fuel fabrication [123].

Spent fuel long-term toxicity can be greatly reduced by adopting advanced nuclear fuel cycles that foresee the extraction of minor actinides (MA), namely Am, Np and Cm, later introducing them in fresh fuel for their transmutation in fast reactors [28]. This can be achieved in homogeneous mode, by diluting a low content (a few % of heavy atoms) of MA in conventional fast-reactor fuel, exploiting the structural similarity of the various actinide oxides and their reciprocal solubility [28]. This has minimal impact on reactor safety parameters and facilitates qualification [28,124], but implies that all fuel elements will contain some MA. Heavy shielding and remote handling will therefore be necessary for fuel fabrication and assembly production, because MA exhibit high neutron emission, thermal power and toxicity. In another concept, the heterogeneous mode, MAs are located only in specific assemblies that are placed at the periphery of the core of the reactor, which minimizes the perturbation of the behaviour of the core [28,124]. In this case, the number of MA bearing assemblies remains limited and these may be manufactured in dedicated plants. In both cases, however, a large R&D effort is required to ensure MA-bearing fuel qualification.

In the longer term, the adoption of mixed U and Pu carbides and nitrides (denoted as MX = MC and MN) will enable core performance optimisation [109]. These fuels moderate less, thus leading to harder neutron spectra, with shorter doubling times (time to produce twice as much fuel as consumed) [125]. They have similar melting point as MOX, but higher thermal conductivity. This enables operation with a larger margin to melting (safety margin) or with a higher linear power (economic gain) compared to oxide fuel [110,112]. However, achieving high purities in these fuels poses some challenges in the fabrication process [112]. The volatility of actinide carbides and nitrides at temperatures below the melting point, in addition, may complicate Pu multi recycling, if it was proven that the built-in Am component is actually more volatile than the U and Pu constituents [126,127].

HTRs also use fissile element oxides, but in the TRISO form [128]. TRISO stands for TRi-structural ISOtropic particle fuel. The concept is based on the idea that a silicon carbide layer acts as a sort of miniaturised pressure vessel to contain the fission products. The TRISO particle is made of a fuel core that is currently composed of U oxy-carbide (UCO, a mix of U oxides and U carbides); in the future it may contain U nitrides, instead [129]. The fuel core is enrobed in a porous carbon buffer layer, a first pyrolytic carbon layer, a SiC layer, and a second pyrolytic carbon layer, which altogether act as very effective barriers against fission product release. TRISO particles have a diameter of less than 1 mm and are very robust, being designed to resist neutron irradiation, corrosion, oxidation and especially high temperatures. In conventional TRISO compacts the particles are encased in a graphite matrix, which in future systems may be replaced by silicon carbide. The whole system is conceived to avoid the possibility of fuel melt in the reactor under any circumstance.

Finally, in molten salt reactors (MSR) the fuel can be dissolved in the coolant salt, so that fuel and coolant are one single medium. Molten halides (typically fluorides, but also chlorides) are used as carriers of the fissile (U, Pu) or fertile (U or Th) elements [117,130,131]. The fuel synthesis route has thus very little in common with the established solid fuel pellets fabrication. Challenges lay in the optimization of the composition for what concerns neutronics and clean-up conditions. The in-reactor behaviour is also very characteristic of this type of fuel, for example in the following aspects: (i) radiation effects are less important, (ii) thermal transfer depends on fluid dynamics and fluid thermal properties (heat capacity, thermal conductivity, density, viscosity and surface tension), and (iii) the solubility of the fission products in the fuel plays a major role for reactor safety. While many fission products are soluble in the fuel, noble gases and metals are not and need to be extracted during operation. This on-line separation of the fission products, which is needed to allow continuous operation, is a current topic of research. The impact of long-term corrosion towards structural materials also deserves attention.

As a mirror of Table 2, Table 3 lists the different types of fuels and indicated in which systems they are used, including use in current generation reactor, if any.

Table 3. Summary of classes of fuels through reactor generations. MOX = mixed U-Pu oxide fuel, MA = minor actinides, MX = carbides, nitrides, silicides, . . . , TRISO = TRi-structural ISOtropic particle fuel, (V)HTR = very high temperature reactor, GFR = gas-cooled fast reactor, MSR = molten salt reactor.

Type of Fuel	Use in GenII/III	Use in GenIV	Notes
UO_2/MOX pellets	All reactors	Mainly liquid metal (or supercritical water) cooled reactors, certainly in prototypes, including GFR prototype	Vast experience on their use [107], but modifications needed for GenIV (geometry, architecture, microstructure, . . .) [108,109,118,119]. Qualification needed for different coolants.
MA-bearing oxide fuel	None	Prospectively in all fast reactors	Homogeneous vs. heterogeneous modes studied almost exclusively for liquid metal (sodium) cooled reactors [28,124].
MX	None	Long term use (with or without MA) in all fast reactors for higher efficiency and safety margins	Fabrication not trivial [112]. Potential issues in connection with Pu multirecycling [126,127]. Qualification open.
TRISO concept	None (but used in formerly built HTRs)	(V)HTR, GFR	Inherently accident tolerant fuel (see text)
Liquid (molten salt) fuel	None (but used in early prototypes and experimental reactors)	MSR	Totally different type of fuel. Offers possibility of online processing [117,130,131].

2.4. General Materials-Related Issues for Improved Circularity and Economy of Any Type and Generation of Reactors

The materials solutions adopted for light water SMRs do not need to differ significantly from those adopted for standard LWRs. Likewise, the materials of choice for SMRs of GenIV technology, or AMRs, can be in principle the same as those for larger scale reactors. However, this one-to-one translation of materials solutions through reactor scales, which is certainly useful for faster licensing of prototypes and first-of-a-kind reactors, may not necessarily be the best choice in general terms. For instance, Ti alloys may be an option for the vessel and perhaps the internals of light water SMRs [132], because they offer reasonably good mechanical properties (no ductile-brittle transition temperature) and corrosion resistance (no need for anticorrosion cladding in the vessel), interestingly combined with lower activation (remote handling activation level reached after 30–35 years) and lower weight (about 1.5 times less) than steels [132]. The latter two features enable easier recycling and facilitate transport of pre-fabricated reactor parts, respectively. There are, however, downsides: little experience with Ti-alloy use in nuclear environments (Ti is a hydride-former and so prone to delayed cracking) and price (up to one order of magnitude higher than steels). Ti is also penalised by being 10 times scarcer on earth than Fe: even though it belongs to the top 10 most abundant elements in the earth's crust [133], it has been recently added to the list of critical raw materials of the EU [134]. However, in the case of small size reactors the advantages that Ti alloys may bring in terms of transport, handling and recycling might compensate in the long term for its shortcomings. Thus, moving to a different, and so far unexploited, type of alloy, with overall not astonishingly better mechanical or corrosion resistance properties, but with better properties from a circularity perspective, may eventually provide increased sustainability as a balance to higher costs. These are thus variables that acquire ever higher importance and need to be included in the equation for the selection of nuclear materials for reactors of any technology readiness level, including established technologies.

From a circularity perspective, GenII/III reactor LTO is not only an important affordable contributor to progressive electricity decarbonisation [6], but also a move towards better use of materials resources and thus waste reduction. For this reason, GenIII+ new reactor builds and future GenIV systems alike need to be designed for as long a lifetime as possible (generally 60 years are targeted), in both cases calling for suitable design criteria in terms of materials performance, although of course the task is made easier by previous component operation experience. In this framework, any materials science-driven technology that is able to increase the lifetime of components for any reactor generation is part of the overall move towards improved circularity and increased sustainability, with the non-negligible side effect of significant economic benefits.

Both LTO of operating reactors and extended lifetime cycle of future ones demand the ability of guaranteeing the integrity of all parts of the plant for the required operation time, by timely repairing or replacing any repairable or replaceable piece and by monitoring the overall health of materials and components, which also has crucial safety implications. Traditionally, this has been done through planned inspections and subsequent testing of key component materials. The surveillance programme of RPV steels, with pre-located capsules containing specimens to be periodically extracted for mechanical testing is the earliest and best example of this practice [135]. The increasing use of non-destructive examination (NDE) techniques for monitoring also RPVs represents a crucial move towards continuous monitoring [136,137], valuably complementing and, eventually, partly replacing planned inspections and destructive testing. Modern approaches of this type are based on the application of optimised multi-parameter methodologies for the in situ characterization of degradation in materials and components through sensors, thereby capturing the material properties ("material DNA") right from the start of its development, including control of the manufacturing procedure, until its end of operation [138–141]. Their interpretation more and more often requires the help of artificial intelligence for pattern recognition [142]. This approach contributes crucially to a thorough plant lifecycle assessment and resonates and connects with the digitalization trend in the nuclear (and not only) industry, which also involves the development of digital twins for the key plant components [143]. These are virtual copies that, by combining in situ data collection with either physical or data-driven computer simulation techniques and models (see Section 3.2), allow the behaviour of the component in operation, or under off-normal conditions, to be anticipated, thereby optimizing its functioning, while enabling timely interventions and, if needed, replacements, whenever required [144].

Importantly, the development of robust technologies that are capable of determining in-service material performance, not only by monitoring, but also through modelling, depends on both model accuracy and data reliability. Hence, there is a need for collecting reliable experimental key data, which need to be captured in a consistent manner under realistic operation conditions, or else to provide physical information on materials behaviour, to be used to feed suitable models. In the case of operating reactors, there is clearly an interest, in this context, to harvest service-aged material to enhance the knowledge base. In the case of future reactors such data collection process needs to be foreseen and designed according to modern conceptions. The corresponding models can be both physical and based on data-driven approaches, using artificial intelligence (see Section 3.2). In both cases and especially in the latter, the inherent consistency and the appropriate collection, storage and management of data are crucial. Non-destructive methods for materials characterization of components during operation, or in experimental *operando* conditions, through sensors, can be helpful to provide also such key data, provided that they can be translated into quantities that the models can handle.

The repair, replacement and fabrication of component parts, especially when these are not classical spare parts and/or possess complex geometries, may benefit from modern manufacturing techniques, such as 3D printing [145,146] and hot isostatic pressing (HIP), which are also used in combination [147]. Additive manufacturing (AM, 3D printing) is suitable for components of complex geometry, but limited size, for which suppliers may be difficult to find. HIP allows shape and material homogeneity and composition to be controlled and is especially suitable for heavy components (elbow pipes, pipes with integrated nozzles . . .). Both are extremely powerful and open the way to revolutionary ways of not only replacing, but also fabricating parts and components, or even a complete reactor [148]. In this way, the supply chain of repaired or new components according to specifications would be significantly improved or even by-passed. However, the safety constraints that apply to nuclear installations require that suitable qualification paths and standards are developed, because a 3D-printed material, although chemically identical to the reference one, will generally have significantly different microstructural features and thus different macroscopic properties [146].

NDE and advanced manufacturing, when applied to the concept of SMRs, open the way to envisaging largely automatised, robotic, intelligent systems that, in addition to being small, compact, factory-fabricated and transportable, are also able to self-monitor the health of their components and replace them autonomously on-the-fly. While still largely speculative, this scenario is not totally science-fictional. These concepts remain valid for current and future generation reactors alike.

3. Nuclear Materials Science and Engineering Approaches: Towards a Paradigm Shift

The ability to foresee as reliably as possible the lifetime of materials and components is clearly of high importance for their optimal use from the point of view of economics and sustainability, as well as for the purpose of licensing reactors of any technology. This requires predicting the moment when, due to the action of degrading agents and processes, the material used to manufacture the component is likely not to be any more suitable for correct operation, or becomes unsuitable to face off-normal conditions in case of an accident. For this we need to know how the properties of the material change after exposure to operational conditions, starting from known initial properties that depend both on chemical nature and microstructure and/or architecture; the latter being determined by the manufacturing process. We also need to know how a component made with a material with those properties will function under given conditions. This knowledge enables the design lifetime to be defined and the maintenance and replacement to be planned, as well as the eventual re-use or recycling to be guided, with all the related safety, economic and sustainability consequences. This knowledge also enables demonstration of the safety and functionality of the component in the process of licensing, or in connection with LTO [149].

In order to obtain this knowledge, materials scientists and engineers dispose of a number of methodologies and approaches that have traditionally enabled materials to be tested and characterised by measuring their properties with appropriate techniques (often, but not always, standardised) under various conditions: as-fabricated, exposed to different degrading agents and during operation, as well as at the end of its life. Testing and characterization techniques may be destructive or not and generally require appropriately prepared specimens. The data obtained in this way are then transferred to models that enable their rationalization and interpretation, allowing interpolations and possibly also extrapolations. It is mainly the models, which can be empirical, theoretical or a mixture of them (e.g., data-driven models), that guide component design, maintenance and replacement plan, minimizing costs while maximizing safety and efficiency, possibly taking into account also all aspects related the optimization of their whole lifecycle. Importantly, these approaches and methodologies are applicable also beyond the classes of materials that are the focus of the present paper, e.g., they are applicable to concrete and polymers, as well as to functional materials, that are also of importance for nuclear power plants.

The above-described way of proceeding, in which the observation of the materials performance under a variety of conditions, unavoidably limited to relatively few data, was the main ingredient in their qualification and licensing, corresponds to the "observe and qualify" paradigm, where models are used *a posteriori* to guide actions. This practice is still used today and will continue to be used, but it must progressively undergo a shift to the "design and control" paradigm. The latter is based on the key postuilate that good models based on physical understanding of processes should also be able to provide paths towards improved materials. These are materials that, because of their inherent properties and the selected manufacturing procedure with respect to a known reference, enable the component design lifetime to be increased, the intervention for maintenance and replacement to be minimised and the possibility of re-use or recycling maximised, while possibly using non-critical chemical elements. Modern materials science approaches, therefore, pursue a new "design and control" paradigm, which inverts the process by asking first the question of how materials should be selected, improved and manufactured, i.e., designed, in order to optimally fulfil the requirements imposed by the targeted operating conditions, i.e., by controlling their performance. This change of paradigm, applicable to all classes of nuclear materials, including those not addressed here, is illustrated in Figure 3.

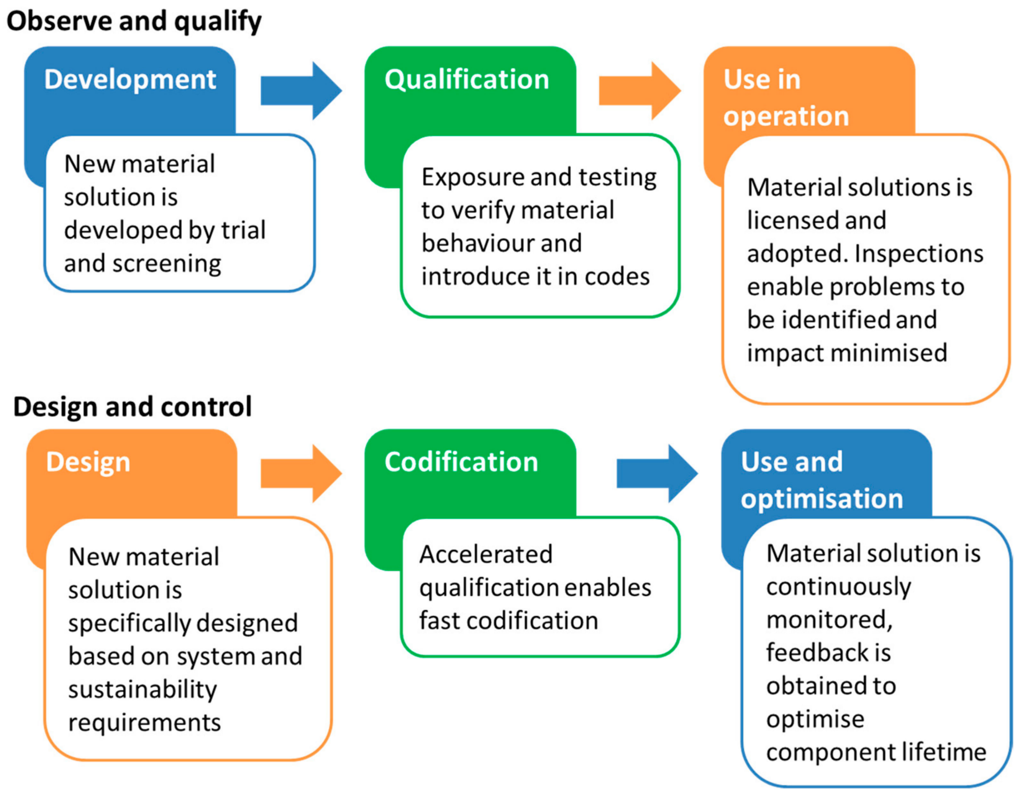

Figure 3. Schematic illustration of the "Observe and Qualify" and "Design and Control" paradigms. The colours help to show that in the latter case the point of view is inverted: material solutions are designed based on operational and sustainability requirements.

The related materials science and engineering practices remain the same in both cases, namely, in logical order: development, qualification and monitoring, with the common denominator of data management and modelling. In what follows, however, qualification is addressed first, because in the traditional "observe and qualify" paradigm nuclear materials have been first identified based on previous experience and then qualified for use in the relevant environment and monitored in it, subsequently deriving suitable models, rather than developed *ad hoc*. Development is the last practice to be analysed, being the crucial one towards "design and control". Data management and modelling are mixed. Moves towards the new paradigm are proposed and discussed throughout.

3.1. Materials and Components' Qualification

Materials and components' qualification means "generation and maintenance of evidence to ensure that they will operate on demand, under specified service conditions, by meeting system performance and safety requirements". Crucially, the qualification is made before the material is used and the component installed, to enable the design of the component itself with sufficient *a priori* guarantee that it will respect performance and safety requirements. Qualification is thus the pre-requisite for the establishment of rules for the design of components, which are collected in design or performance codes [150–154], according to the best available engineering practices and scientific knowledge. The related research is defined as pre-normative, with reference to the goal of establishing norms and standards. This qualification needs to be completed for each material of interest for applications or, in cases that are more and more frequently encountered, for whole components or assemblies. For instance, fuel elements need to be qualified in their entirety for the target environment and conditions and require, for design and safety purpose, the development of fuel performance codes [152–154]. These enable the simulation of the behaviour of the fuel element in the reactor from the thermal and mechanical point of view, as well as its evolution overtime, as functions of irradiation and thermal parameters in any condition: normal, incidental and accidental. The description of the very complex relationships between these parameters and the evolution in time requires appropriate models. It is considered that better models can be produced by shifting from currently used fully empirical correlations to partly or totally physical/data-driven models (see Section 3.2). In addition, modern techniques of component fabrication (AM, HIP) inherently require the qualification of the whole component, because the properties of the material become linked to the method and the process used for its fabrication. This requirement involves the development of suitable standards, that currently only partly exist, especially in the case of next generation reactors and relevant materials [155].

Design codes include guides for the introduction of a new material in them, where a “new material” is not always really “new”: it can also be a known one that was never used before for a given application and thus needs qualification for the conditions to which it will be subject, i.e., the conditions to which it is going to be subjected are new, rather than the material. Alternatively, the “new material” may be a one that was already used, but was fabricated according to different standards or adopting different processes, as is the case of advanced manufacturing. These guides to introduce new materials in codes are sorts of checklists of the type of information and properties that need to be provided through qualification and pre-normative research, together with indications about how to execute the relevant measurements and tests, referring to standards that are developed for this purpose by dedicated organizations. These give prescriptions on how to conduct tests and often also on how to analyse data, to assure that the measured material properties are independent of who performs the test and where. In some cases, however, for operation in environmental conditions and parameter ranges that concern specific new systems, the design codes may fall short and require extensions. For instance the RCC-MRx design code [151], which was developed in France to support specifically the SFR technology, has been recognized as the most appropriate design code for all European GenIV prototypes. It covers the design and construction of components for reactors that operate at high temperature, including auxiliaries, mechanisms for examination and handling and irradiation devices. It also includes specifications on manufacturing. However, it does not advise on rules for environmental effects, with the exception of thinning by corrosion. It does not cover high temperature ranges for GFR and (V)HTR, either. Moreover, the reference operational life for material property curves and design rules is 40 years, while the goal of increased sustainability requires extension to 60.

Filling these gaps for a given material requires that dedicated experiments are performed to collect comprehensive and reliable sets of relevant data. In the case of nuclear core materials irradiation experiments need to be included, as well. Materials need to be exposed to specific environments in suitable and often expensive infrastructures, such as autoclaves and loops, or bespoke facilities for irradiation, if possible up to the time or dose expected in service, else getting data that can be possibly extrapolated. For fast reactor systems this should ideally happen in facilities with the correct neutron spectrum. In their absence—as is currently the case in Europe—Materials Testing Reactors (MTRs) are used.

These are, however, characterized by a predominantly thermal neutron spectrum, which limits safe extrapolation to different spectra and higher doses. This problem, which hinders full qualification for GenIV reactor materials, is even more burning for fusion, because the neutron spectrum is in that case significantly different, with a 14 MeV peak that has significant consequences, especially in terms of transmutation. It becomes therefore necessary that a bespoke facility should be built to irradiate under fusion-relevant conditions, which is the purpose of the IFMIF-DONES project [156].

The level of degradation after or during exposure needs to be assessed in terms of changes of properties of engineering interest, by testing and examining these materials, using a series of suitable testing methods. In order to cover most conditions through testing, particularly those with safety implications, the qualification process may currently last for decades. The return of experience from previous use, when applicable, does reduce the qualification time. However, in several cases this process is system-specific, thus the return of experience may not be fully of relevance. Moreover, new and bespoke standard procedures may need to be developed to execute the exposure, the characterization and the tests in new environments. Furthermore, the qualification of a new material, or material combination, in its baseline version is not sufficient: efficient procedures for joining pieces made of that material need to be developed and equally tested and qualified (One of the important advantages of fabricating components using advanced manufacturing methods is that welds and joints can be avoided, as the component is given a shape while the material itself is produced. However, this advantage should not be offset by internal stresses and porosity). Finally, both new materials solutions and joining procedures are typically developed in the laboratory, but, crucially, before the solution can be actually adopted in commercial plants, there needs to be an industrial production upscale, which is not always obvious. In particular, upscaling may imply *de facto* changing some of the features of the materials solution that was developed in the laboratory, potentially requiring further qualification. Eventually, the data that are gathered for each code-candidate material through this long and expensive procedure need to be rationally translated into robust design rules for components, or laws and models for the assessment of fuel performance.

The qualification process would greatly benefit from the development of accelerated exposure and testing procedures, which would reduce the associated time and costs, with significant impact on innovation and thus economics. Identifying them, however, is not simple, because their relevance to real operating conditions needs to be proven. Advanced modelling (Section 3.2) is crucial for accelerated qualification, as it provides the required links between properties and should enable the effects of degradation processes to be more precisely assessed, based on physical insight. Likewise, monitoring (Section 3.3), such as in the case of RPV surveillance [135], is crucial to ensure the integrity and functionality of materials and components while in operation, even in case of partial failure of the qualification procedure, as well as to provide an *a posteriori* feedback to the design rules. Yet, monitoring is possible only when the reactor fleet or at least a prototype/first-of-a-kind has been deployed. Thus monitoring does not generally support materials and component qualification, although it does compensate for the fact that not all possible combinations of conditions could be explored *a priori*.

With a view to making qualification more efficient and affordable, and possibly accelerate it, the concept of “test-beds”, supported in Europe for example in the case of nanomaterials [157], should be pursued and adapted to the case of nuclear materials or, more generally, materials operating under harsh conditions. Test-beds are integrated platforms for conducting thorough and replicable tests on (new) materials, according to an established protocol that is specific for the target application. These platforms may or not be physically in the same place, i.e., they can also be the result of properly structuring coordinated characterization using different techniques by different specialised laboratories. The definition provided by the EU commission is: “entities that offer access to physical facilities, capabilities and services required for the development, testing and upscaling of advanced materials in industrial environments” [157,158]. The key is that they should offer any type of customer the possibility to obtain an exhaustive and integrated characterization, under or after suitably representative exposure conditions, of materials belonging to the classes of interest for the target applications. Single-entry integrated platforms of this type, if sufficiently flexible, can help making the qualification steps of baseline and joined materials shorter and more affordable, including support to industrial upscaling.

3.2. Advanced Modelling and Characterisation

The previous section makes it clear that exposing materials to real conditions costs time and money and requires infrastructures. Moreover, in practice, those that can be explored correspond to simulations or approximations of real conditions and data can never cover all ranges. Exposure times or doses comparable with the lifetime of the reactor are only rarely accessible, or they may be accessible at higher dose rates using MTRs, as is customarily done to evaluate RPV steel embrittlement [76,159,160]. The combination of effects and their synergy is also difficult to simulate in a laboratory. Finally, until the system is operated, no feedback can be obtained through materials health monitoring (Section 3.3). Extrapolation of data is therefore unavoidable, but purely empirical extrapolations have limited reliability. Relying only on the observation of the materials performance under a variety of conditions, unavoidably limited to relatively few data, as main ingredient in their qualification and licensing corresponds to the "observe and qualify" paradigm. Shifting to the "design and control" paradigm requires the help of advanced models. These can be of two complementary types, as described in what follows.

Advanced physical modelling through numerical simulation and modern materials examination methods are at the heart of the "design and control" paradigm. This paradigm is indeed made possible thanks to the vast increase that computational power experienced over the last decades, combined with ever greater power of techniques for microstructural and micromechanical characterization of materials, which enable in-depth observation and testing at all scales [161–163]. This approach is expected to become increasingly robust, initially only underpinning, then gradually improving the traditional empirical approaches that are still used, e.g., in fuel performance codes [152–154] or in dose-damage correlations for LWR vessels [76]. The "design and control" approach bears the promise to significantly enhance our predictive capability, by enabling the physical description of the evolution in time of both the microstructure and the microchemistry of materials exposed to irradiation and/or high temperature and/or coolants. The output of these models acts then as input to meso- and macroscopic length scale models, in a multiscale modelling framework and spirit, thereby enabling prediction of the changes experienced by the materials properties in operation. Since the modelling tools are generally computationally costly to run and often use parallelised software, the use of high-performance computing (HPC) can be a crucial asset; although in reality the bottleneck to physics-based model development is not only computing power, but mainly the correct identification and parameterization of all important physical mechanisms [163,164]. Eventually, correlations of fast application such as those used for RPV steels or performance codes such as those used for fuel should be able to make use of the background information that these models provide, using better parameters and models and including more correct underlying mechanisms, possibly under a single platform [165,166].

Physical models require suitable data for calibration and validation, from so-called modelling-orientated experiments. In these, materials are exposed to external factors, as for qualification purposes, but the objective here is to better understand mechanisms, by separating variables and effects, rather than to measure engineering properties [162,163,167]. In experiments of this type, key variables, such as temperature and irradiation dose or dose rate, are accurately controlled and varied over sufficiently wide ranges. For this, specific exposure facilities are needed, especially for irradiation, and the use of charged particles (ions, protons, electrons, . . .) can be a valuable and affordable tool (some caveats are discussed in Section 3.4) [168–170]. Next, microstructure and microchemistry characterization are essential parts of modelling-orientated experiments. The combined use of various modern characterization techniques (a list of which will never be sufficiently exhaustive) is crucial, because each of them provides complementary pieces of information, which are all indispensable in order to actually take advantage of the added value of modelling-orientated experiments [162,163,167]. Suitable mechanical characterization is equally important, including micromechanical experiments from specimens at single grain scale (nanoindentation, micro-pillars, . . .), often the only possibility in the case of specimens irradiated with charged particles, due to the latter limited penetration [171]. Moreover, mechanical tests addressing uni- vs. multi-axial load, cyclic load, relaxation, load sequence, non-proportional loading, etc., in correlation with the observed microstructure, are of interest, depending on material type and purposes and models to be developed. These experiments are invariably delicate to perform and may be longer than, and almost as costly as, those performed for qualification. They provide, however, a higher level of fundamental physical understanding, as opposed to the collection of engineering data for the production of correlations that is typical of traditional qualification procedures. They thus clearly contribute crucially to the paradigm shift towards "design and control".

The main current limitation of physical computational models is that they still have difficulties to take into account, at all scales, the effects of the complexity of materials chemistry and related mechanisms of degradation, even more when the interaction with the environment (e.g coolants) has to be accounted for. This difficulty is likely to require significant time and effort to be overcome. An alternative path has therefore recently started to be intensively pursued, which consists in using modern digital techniques such as artificial intelligence (AI)—also used for the analysis of data obtained from materials health monitoring (Section 3.3)—to extract relevant materials features from large amounts of data: so-called (big) data-driven modelling [172,173]. These techniques make the best of the data that can be made available, by identifying complex correlations between, on the one side, the parameters that define the materials or the components (e.g., composition and fabrication features), as well as the exposure conditions (e.g., temperature, exposure time, radiation dose and dose-rate, . . .), and, on the other, the final properties of interest. This is achieved by providing a large amount of examples, on which the method is trained. The accuracy is then tested by contrasting the outcome of the AI scheme with data that were not used for the training. These sophisticated algorithms turn out to be often very powerful. The specific example in the nuclear materials field where this approach is being applied with some degree of success concerns correlations for RPV steel embrittlement versus neutron fluence and other variables [174–176].

One of the main problems with data-driven modelling procedures is that they are too often blind: the AI produces in most cases a sort of "black box" transfer function between input and output, *a priori* devoid of any physics (even though sometimes this procedure manages to improve also our physical understanding [174,175]). The more data are available, the higher are the chances that the procedure provides probative results, although it remains dangerous and unwarranted to rely on extrapolations [176]. In the case of RPV steels, a large amount of data is available from surveillance and MTR experiments, thus this approach is especially promising [174–176]. However, this situation is not necessarily common in the nuclear materials field. In general, the number of data that are available for pre-normative research and for modelling, from exposure to a variety of environments and irradiation conditions, is limited, due to the high cost and relative scarcity of relevant irradiation experiments. Thus, a completely blind approach based on "big data" analysis techniques is of hardly any use in the case of nuclear materials, for which data are in fact generally rather "scarce" than "big". AI methods that are able to find logic in scarce sets of data do exist (few shot learning) [177]. They are based on the multifidelity concept, i.e., whenever high fidelity data are missing, pseudo-examples based on lower fidelity data are used as complement, with appropriate weight. Their application relies on the availability of various and different ways to obtain data and reaches its highest efficiency when input is received from both experimental high quality data and data of different fidelity level, e.g., coming from physical models. It is also believed, and has been shown in some cases, that the inclusion of microstructural data from advanced characterisation in the set of input variables greatly improves the predictive capabilities of AI algorithms, because of the added physical content that this involves [178]. Therefore, in the field of nuclear materials and components, the marriage between data-driven and physical modelling (hybrid models), combined with advanced microstructural examination, is likely to be the most promising path to follow. Other methods to reduce the "black box" effect inherent to AI, for a different application, are discussed in the next section.

3.3. Materials and Component Health Monitoring

Until recently, non-destructive testing and evaluation (NDT&E) were mainly used to detect defects in components and products as part of quality assurance procedures [179,180]. Thus, NDT&E have been often designed, for many applications, as an afterthought, instead of being an integral part of their design and manufacture. As an example, an early overview on the NDT&E versus linear dimensions of microstructure and defects relevant for material strength and toughness is given in [181].

Today, NDT&E do more than purely detecting and locating defects in components: they address the characterization of material properties and their progress and can therefore contribute to all stages of the product life cycle, from the development of materials and products, to cover their maintenance, repair, and finally recycling [182,183]. Last but not least, the development of sensors that are able to capture microstructural patterns emerging from production processes [184] and to combine them in the form of individual fingerprints is also part of NDT&E: this corresponds to a sort of "product DNA" that can be deposited in "digital product files".

NDT&E methods for materials health monitoring have the advantage of being able to characterise the progressive change of the material properties of the same specimen in *operando* conditions. They can also be applied to actual components, again also in *operando* conditions. The key for their application is that macroscopic physical properties and microscopic effects are correlated based on physical principles [185]. Depending on their physical principles and applied sensors, NDT&E methods can provide local or volumetric information about the material or component condition [185,186]. Moreover, many of them can be used on activated materials (under harsh environment) and in situ [187,188]. However, tests performed non-destructively do not generally determine directly the material properties as they are measured in destructive tests. To quantify the material properties non-destructively, measured parameters/features must be first correlated with the material properties of interest, which are customarily measured destructively [185,189].

Smart NDT&E systems should enable the collection of, and access to, essential comprehensive data of materials/products along their entire lifetime at different scales, starting with their development (in the lab) and ending with their end-of-life over production and operation. Moreover, innovative NDT&E methods that include cognitive, auto-adaptive sensor technologies may enable the understanding of the physical mechanisms that determine the response of the material under given conditions of manufacturing or operation [190].

Intelligent NDT&E devices may collect experimental reliable key data during laboratory materials characterization, until industrial inspection of in-service components, and predict the progress of material properties with high accuracy. For this to happen, each change (intended or not) of the material properties of a product along its lifetime must be detected and stored in a sort of product memory. To allow an as comprehensive material characterisation as possible, multi-parameter/multi-NDE methods approaches are needed. They enable materials characterisation similarly to having different human-senses [190–192]. A current limitation of the multi-method approaches is the unavailability of uniform data formats for data obtained by different NDE techniques. An additional limitation is caused by the risk of obtaining big datasets that contain many irrelevant data. AI algorithms of the same type as those used for data-driven modelling (Section 3.2) are thus equally helpful here for data collection and analysis to build models based on collected data and make predictions or take decisions [193], provided that the training data are appropriately treated.

The application field of AI can be roughly divided into two groups, supervised and unsupervised learning, to which the semi-supervised group may be added [194,195]. They can be applied to different stages in the NDT&E: data collection first, than data analysis or prediction of the targeted material property. In supervised learning, so-called targets (the variables to be predicted) are available in addition to the features (the independent variables). The model aims to predict the targets based on the features, in full analogy with the data-driven modelling of Section 3.2. This is by far the most frequent type of application in materials science. The simplest example of supervised learning is multiple linear regression analysis ($y = m_1x_1 + m_2x_2 + \ldots + m_nx_n + b$) [192], where the features represent the independent variables ($x_1, x_2, \ldots$) and the target (y) represents the dependent variable. AI supervised learning models generally necessitate large databases for their training and for their validation. In the case of NDT&E there is no issue of scarce data, as in nuclear materials data-driven modelling (see previous section), but rather of guaranteeing the relevance of the training data, removing signals from faulty sensors or spurious signals. In unsupervised learning the goal is to draw conclusions about the input data, rather than predicting the corresponding output variables. This approach searches for patterns in data that have not been detected before. For instance, it may identify ways of grouping unlabelled data, thereby providing a data classification. The algorithm thus identifies trends of potential use and interest to rationalise the dataset, so available data can be presented in a novel way. Thus structures in the data are recognised and the aim is not to predict the target property, but to present the training data in a more comprehensible way (clusters) for humans or subsequent supervised learning algorithms [190]. Curing the training dataset to avoid implausible data, like errors, outliers or missing data is customary in all cases, also in supervised learning, i.e., the collected data always need to be pre-processed [195], the volume of data, the uncertainties associated with each data value, as well as their heterogeneity, all being important aspects of data pre-processing. What unsupervised algorithms do is to help in the pre-processing, by reducing the number of dimensions of a multidimensional feature space, through rotation and subsequent projection onto so-called principal axes, thereby removing redundancies and irrelevant data, without significant loss of information [195]. By applying this approach, future NDE systems will be enabled to collect only relevant materials data. If, after the cataloguing, the experimental data acquired are not enough for performing reliable trainings, then the quantity of data can be increased artificially, without the need for large amounts of specimens, thanks to the prior clustering. Thus, specific data augmentation techniques based on unsupervised algorithms can be designed in order to obtain a sufficiently large, and optimised, database. An example of unsupervised learning is principal component analysis [192,195]. High-dimensional and correlated NDE datasets have to be analysed in terms of outliers and missing data and mapped in a reduced, decorrelated and thus interpretable feature space, using unsupervised machine learning algorithms. This ensures the ability of the model to be developed to deal with possible failures, inaccuracies and errors (i.e., outliers, missing data), thereby reducing the "black box" component.

The combination of supervised and unsupervised ML-algorithms can be used to extract relevant features from NDT&E and so build models for predicting material properties, much in the same way as in data-driven modelling (Section 3.2), although using approaches that are specific for this type of analysis. Once the data pre-screening is performed, a prediction/modelling of the material properties of test-specimens can be carried out. NDE data, in combination with the associated reference data and the use of supervised machine learning algorithms (e.g., linear and nonlinear regression models), are then used for explainable robust model building, from which reliable non-destructive predictions of the targeted material properties can be determined.

AI algorithms embedded in NDT sensors will thus enable the collected data to be pre-processed and the key relevant data to be selected. AI-based multi-parameter NDT&E

systems (merging different NDE sensors and AI algorithms), which can predict individualised material properties, can be used as an added-value option in the framework of materials development, product design, manufacture, predictive maintenance and traceability of material properties for secondary raw materials. They can provide reliable key experimental data collected non-destructively in all stages of the entire product life cycle [196,197].

3.4. Development of Optimised or New Material Solutions

Appropriate system and component design may contribute to mitigate the harshness of the conditions to which materials are subjected, thereby enabling sufficiently long lifetime in operation. However, no design can fully compensate for inadequate materials properties, if the reliability of the component and the availability of the system remain too low to be economically viable. This is the case for most GenIV systems, for which currently no readily available materials or material solutions enable the target operating conditions for commercial power plants to be fully sustained (see Sections 1.1, 2.2, 2.3 and 3.1).

Materials with better initial properties and performance in terms of resistance to degradation enable safer, more efficient and more economical design of installations. Advanced manufacturing techniques and processes, such as AM and HIP, might also help increase the performance of components and enable their repair or fast replacement. Both ways, component or installation lifetime is increased and shutdowns become less frequent or shorter, thereby improving the availability and the economy of the installations, as well as their sustainability, because increased component lifetime leads to better use of resources and minimised environmental impact. The push to find material solutions with improved performance in operation is therefore strong and the equation to find the best materials solutions should also include variables such as criticality of raw elements, component monitorability (Section 3.3) and materials recyclability (or possibly re-use), as well as safe and easy disposal when this becomes unavoidable. The forces that oppose the push towards the development of new materials solutions originate, in the case of new systems, from the need for designers to identify rapidly suitable materials that are already, or can be readily, codified, so as to enable timely design. In the case of already deployed systems, the "counter push" comes mainly from the (cost of the) industrial production transformation that the new solution implies (industrial upscaling and supply chain). In both cases, the need to be convincing with regulators for swift licensing is an issue.

New materials solutions may be: (i) existing materials that are expected to be suitable for given conditions, or more suitable than previous ones, or simply cheaper, but were never used before for those conditions; (ii) materials with purposefully or expectedly improved properties and performance, thanks to, e.g., tuned composition or revised architecture; (iii) materials of the same type as those already used, but produced or joined according to different standards, processes or methods; (iv) combinations of the previous two cases, or coupling of different known and new materials, to better mitigate degradation due to specific agents (e.g., coatings against corrosion); (v) entirely new materials solutions that were developed with targeted properties for a specific use. In practice, the last case, which best corresponds to the "design and control" paradigm and appears at first sight as the most appealing one, is by far the least frequent one.

Each time a new material solution is proposed for a nuclear reactor, a long and costly process of full qualification and codification is required (Section 3.1). Thus, qualification steps can currently be taken only for a reduced number of promising materials, which have emerged from a selection based on a previous screening. This is currently doable in practice only for very few candidates, generally selected based on existing knowledge. The screening is performed essentially in the same way as the qualification of materials, i.e., by exposure and testing (the "observe and qualify" paradigm), but here the goal is not to fully define the design rules for licensing and construction: it is rather to give a first assessment of the behaviour of the few candidates, so as to identify the most suitable one(s), on which to focus attention. Thus typically a small set of properties of interest is selected to be measured, after exposure to a reduced set of representative and, especially, affordable conditions. However, even these small sets may correspond to significant work and cost, particularly when neutron irradiation is involved. There remains a certain probability that all materials in this small set (sometimes a set of only a couple of materials) have to be discarded at some point, because of some inacceptable behaviour under conditions of relevance for the target system. Clearly, this is a risky and inefficient way of proceeding, which eventually may lead to using a non-optimal materials solution, simply because it is the one for which, after several years of work, there are more or less sufficient data for codification and therefore design of the component.

In order to explore the performance of materials under irradiation for screening purposes, charged particles that would be of questionable use for qualification can be a convenient method [168–170]. Charged particle irradiation is significantly cheaper and variables such as temperature and dose are easier to vary and control (not so dose-rate, though). This enables a wider spectrum of parameters to be more affordably explored as compared to neutron irradiation, although at the price of only affecting a surface-close layer of material. The latter limits the possibility of characterization to a few microstructural examination techniques, which cannot be of bulk-type. Thus, mechanical properties cannot be assessed using the same approaches as for neutron-irradiated materials. Moreover, contrary to bulk-techniques for mechanical testing, no good practices are fully established for those applicable to charged-particle irradiated specimens, e.g., nanoindentation [171,198]. Finally, serious issues of transferability to neutrons exist, because charged particles are injected at higher dose rate, have different energy spectrum, generally produce damage gradients in a limited penetration thickness and often inject foreign species, including impurities [168,170,199–205]. Thus, theoretical and modelling work to ensure transferability, and a clear definition of suitable protocols, though already started [206], is still needed in order for charged particles to become fully usable screening tools. Meanwhile, costly neutron irradiations remain necessary for screening, as well.

The lengthy qualification process and the costly screening of new material solutions, combined with the hurdle of licensing, make the nuclear industry often overly conservative and incremental, i.e., there must generally be very strong reasons before changing to a different type of material solution. Changes of materials did happen in the past in the case of GenII LWRs [54,207]. However, "not-too-different-solutions" from those already adopted are generally preferred [54], because easier and less costly to adopt in practice, especially in order to be convincing with regulatory bodies.

To make materials development more attractive, with all the benefits this can bring, the screening procedures need to become less expensive, faster and more efficient, possibly including from the start all the important variables in the searching tool to robustly identify the best candidates that are later worth undergoing full (accelerated) qualification. This corresponds to adopting a full "design and control" perspective. Relying on an efficient and affordable screening procedure becomes even more important now that developing new material solutions does not only concern better intrinsic engineering properties (e.g., resistance to operation at high temperature, to corrosion or to irradiation), but also lifecycle improvement for increased sustainability (less use of critical elements, monitorability, recyclability or re-use ...), i.e., the number of variables to be included in the process of development and the selection of materials solutions is increasing. Finally, the involvement of regulators for safety indications to be taken into account from the start of the development process would be ideally beneficial.

Improving the efficiency of the screening procedures implies addressing mainly three aspects: (i) apply suitable fast fabrication and post-fabrication treatment methods to produce an as large as reasonably possible number of batches of materials, with various compositions and/or architectures and/or microstructures, among which the best candidates need to be selected; (ii) identify experimental methods to accelerate exposure and subsequent testing, by rapidly measuring representative quantities that are considered as good indicators of the expected long term performance; and (iii) make use of advanced characterization and digital techniques as guidance to the development of new materials, by using a quantitative methodology that goes straight to the target, instead of proceeding by trial-and-error, solely based on the (invaluable but fallible) experience or intuition of the researchers involved. The keywords to make these three goals a reality are combinatorial fabrication [208–210], high throughput characterization and calculation [210,211], smart physics-based and data-driven modelling [178,212–215], including automated microstructure recognition [215–219].

High throughput experiments and calculations quickly explore the wide phase space of the variables that characterise the materials to identify the regions of interest. Combinatorial fabrication corresponds to making sequences of samples of a certain type of material, in which variables such as composition or architecture vary according to a large number of combinations (for example, mixing different chemical elements in different proportions). Key target properties are then systematically measured in these samples, thereby obtaining a large amount of homogeneous data. High throughput is achieved if the measurements are fast and easy to repeat, automatically and sequentially, in a large number of samples, which should be small to optimise the process also in terms of use of resources. The measured quantities and the way of measuring them (e.g., after suitable exposure to specific conditions) in microsamples must be representative of the behaviour of the material in operation. To complement the experiments, a large number of relevant property calculations are performed using high fidelity physical methods, such as those based on density functional theory (DFT), implemented in high performance computers (HPC). Finally, AI, specifically machine learning (ML), techniques are applied to analyze the collected data, to establish correlations between the fundamental variables that characterise the materials (their "genes" or "DNA") and the properties to be optimised. As in the case of modelling (Section 3.2) and monitoring (Section 3.3), these digital techniques are used to deduce complex deterministic laws that depend on multiple variables, based on examples provided in the form of large amounts of data. As in the other cases, the quantity, quality, homogeneity and representativeness of the data are crucial (Section 3.5). By collecting data in an iterative fashion, these correlations are expected to enable the identification of the subset of the most promising candidate materials for the target set of properties. These should be looked at with more attention later, using more "traditional" qualification approaches, also from a perspective of industrial upscaling. The test-beds suggested in Section 3.1 are an ideal tool for these following steps.

Accelerated development through systematic screening is eventually best achieved by the creation of suitable integrated platforms in which, with the help of robotic systems, the above described methodology of combinatorial manufacturing and high-performance characterization of materials, as well as AI/ML methods, are incorporated in an integrated and automated way, thereby becoming autonomous materials discovery systems (autonomous materials discovery), as put forward and explained in [218–220], and specifically for nuclear applications in [221]. Platforms of this type, called Material Acceleration Platforms, MAPs [222] are being developed and applied with some degree of success in the case of functional materials, such as for lithium batteries [211], also in Europe (BIG-MAP project [223]), and for carbon nanotubes [224].

The challenge of applying these approaches beyond the existing examples to materials for extreme conditions is daunting. Yet MAPs are preconised to revolutionise traditional materials research and development in the next decade, also in the field of energy materials [225]. The combination of nuclear-materials-dedicated MAPs and test-beds (Section 3.1), therefore, can be a way to boost innovation, the need for which is strongly felt in the nuclear energy field [226,227] (see also Section 4).

3.5. Data Management

Data management is becoming an intrinsic constituent of the mainstream research process in all fields [228–232]. The specific reasons can be many, but the substratal motivations are improved science and greater opportunities for innovation. In the specific case of materials, data management enables the application of modern techniques, such as those described in the previous sections (data-driven modelling, materials health monitoring, autonomous materials discovery, . . .), while facilitating more traditional qualification approaches, where the formulation of design rules for relevant codes is hindered by the scarcity of data. Over past decades plenty of test and measurement data have been generated through national and international research programmes, but these are often difficult to access and retrieve. While web-enabled databases have been and are being developed [233,234], potential data providers often do not add their data there, for three main reasons: (i) they are proprietary data protected by confidentiality and therefore cannot be shared; (ii) there is no sufficient motivation for data producers to spend unpaid time and resources for data upload; (iii) the hard, skilled and time-consuming work of data search, often data analysis and always data adaptation to the format of the databases, is hardly ever considered a task in itself, to be duly funded. Given the cost of generating materials qualification data, however, it seems obvious that appropriate data collection, storage and preservation in suitable repositories, with easy access in full respect of intellectual property rights, should be standard practice. Yet, barriers need to be overcome to make it attractive for data generators and proprietors to put their data in the database. The issue of respecting intellectual property rights is especially thorny: agreements are hard to reach and are often too specific to be easily generalised. International organisations such as IAEA or OECD/NEA may be able to partially help in this respect, by providing pre-existing legal frameworks for data sharing [233]. To help, databases should also offer flexible and adaptable tools, for example to guarantee protection of sensible data while allowing access to the parts of them that can be disclosed, which may not be sensible any more when extracted from the context (e.g., data on pressure vessel embrittlement without revealing the plant); or provide the possibility to apply an embargo to data accessibility for a number of years; and so on. There is also a "chicken-and-egg-type" problem to be solved: it is attractive to spend time and effort to provide data to a database if this gives access to data that otherwise would not be accessible; however, if the quantity of data in the database is minimal, or the data are anyway openly available, this motivation largely vanishes. The issue of unleashing skilled data retrievers can be in principle solved with adequate funding. But an associated problem affects old data, i.e., these may eventually turn out to fail to comply with modern data quality requirements, especially in terms of accompanying data (metadata) that enable them to be reproduced and therefore re-used, or protocols that were applied for their generation. Thus, the retrieval of old data for either materials qualification or model calibration/validation in the future, although important and to be added to the "to-do" list, is alas unlikely to contribute significantly to future advances in materials qualification and development. However, the combination of newly produced data in current and future projects that do enforce suitable data management policies should, little by little, but steadily, succeed in creating a critical mass of data, which will partly enable accelerated materials qualification, provided that suitable and attractive databases are created. Ideally, these should: (i) be user-friendly, i.e., they should not only enable the user to easily access and upload data, but also to "play" with them to address issues of user interest, even several years after the data were generated; (ii) apply clear and flexible, but unbreakable, rules of data protection; (iii) use simple and flexible formats that, as much as possible, match the expectations of expert data producers and are sufficiently clear for less expert data users; (iv) apply clear and strict data quality criteria, while also being able to self-search for new data; (v) connect directly with the software that analyses the data, to by-pass the need for humans to upload new data.

For data-driven modelling to be applicable, not only the quantity, but also the quality and consistency of the data are crucial. AI can find the logic in a set of data only if these have been generated and collected in such a way that such logic exists. Thus they must have been all produced by applying consistent procedures. This is generally broadly guaranteed in the case of standardised mechanical or corrosion property tests, or data coming from sensors that all work and have been calibrated in the same way. Not necessarily so when microstructural characterization, or modelling, data are considered. In these cases, inconsistencies between data may be originated by the different features, limitations and possibilities offered by apparently similar types of instruments or techniques used to produce them, as well as by different operator-dependent procedures or choices of measurement conditions, or as a consequence of different parameters and assumptions that may be used for raw data analysis. Data from different laboratories, therefore, too often cannot be merged [235]. Data of qualitative nature, e.g., micrographs, also pose problems of juxtaposition. Finally, all data must be accompanied by all the important specifications that enable their reproducibility: the completeness of these specifications may be challenging. Before AI methods can be systematically used to include microstructural examination results as data-driven modelling variables, therefore, there is a need to define accepted good practices, protocols and possibly standards for the application of microstructural techniques, as well as for the analysis of their results. Furthermore, consistently complete and consensual data formats need to be established. This should allow full inter-laboratory comparability and provide high guarantee of reliability, reducing scatter and uncertainty, irrespective of the number of data that can become available. This process of standardization, or at least definition of protocols, which needs to be extended to microstructural characterization techniques and relevant data format, is also essential in view of developing MAPs (Section 3.4), because only standardised characterization procedures can be automated, while only interoperable data can be effectively used to make conclusions based on data analysis. Defining standard good practices and formats, however, needs to be extended to all existing techniques and requires consensus amongst the experts, therefore being a task in itself.

It is important to emphasise that the establishment of good practices, protocols and possibly standards for (materials) data is a general problem, which concerns all technologies, and not only for the part that concerns materials. It is thus inherently a cross-cutting issue, irrespective of the target application to materials. The FAIR (Findable, Accessible, Interoperable and Re-usable) Guiding Principles for scientific data management and stewardship [236,237] are of universal application. Interoperability and re-use require consistency of the data coming from different laboratories and to facilitate transfer between different information systems. Standard formats for materials data need to be established in order for the highly interconnected information and communication technology infrastructures that have emerged in recent years to become effective in appropriately storing data and ensuring their availability for the purposes of future re-assessment.

4. Discussion

The expression “innovative material solution” has no unique interpretation: for a researcher to innovate is to make something new, for a policy-maker to innovate is to put a new product on the market. In the case of nuclear materials, the situation is especially ambiguous, because a new material solution proposed by researchers with promising properties for a given application clashes with either an industry (thus a market) that might be reluctant to use it, or with the fact that the application is a reactor system that does not exist, yet, thus cannot have a market, yet. In this context, what is, really, an “innovative nuclear material solution”? It should be interpreted as one that “enables significant improvements in reactor design and operation”, for instance leading to increased safety and efficiency, enhanced flexibility and/or prolonged component lifetime [221], as well as potentially cost abatement, irrespective of whether it actually rapidly accesses a market, which in the nuclear field often does not exist, yet, or is limited.

Having given this definition, how are innovative material solutions for nuclear energy created and adopted? It happens in four steps, some of them partly overlapping: (i) adoption (if already available), development, or possibly discovery, of new materials solutions, which often are improvements of the features of existing solutions based on designers’ requirements or declared industrial needs; (ii) industrial upscaling of new materials solution’s fabrication, including joining, to make a supply chain possible; (iii) materials solution’s qualification for the target application to enable design, licensing and eventually construction; (iv) application of material and component health monitoring for optimised lifecycle. The enablers for all these steps are modelling in all its forms and supporting digital technologies, i.e., high performance computing, artificial intelligence, digital twins, . . . , together with appropriate data management. The imperative to foster innovation is that all these steps should become easier, faster and cheaper. The description of the various nuclear materials science approaches in Section 3 suggests that:

- The creation of integrated test-beds dedicated to nuclear materials, and in general materials for harsh operating conditions, can be an effective pathway for accelerated materials qualification and industrial upscaling, based on coordinated exploitation of existing and future facilities and infrastructures at the service of both industry and research.
- Hybrid models that combine physics-based and data-driven approaches, e.g., making use of few-shot learning techniques, can be an effective methodology for nuclear materials, with the potential of optimally blending the capabilities of by now "traditional" multiscale tools and approaches (the development of which has absorbed much effort in the last few decades [165]) with recent data-driven empirical trends.
- Current NDE&T systems complement more traditional characterization methods to monitor the progressive change of material properties over the whole component lifecycle. Multi-parameter-based approaches combining different NDE techniques efficiently characterize materials' properties ("material DNA") similarly to having different human-senses, thanks to AI algorithms that remove irrelevant or spurious data, best blended in cognitive sensor systems, for advanced digital twin concepts.
- The development of MAPs dedicated to nuclear materials, or more generally materials for harsh operating conditions, is an ambitious, but extremely promising goal to apply a "design and control" paradigm for materials screening and perhaps discovery, with high potential to boost innovation in a field that needs it [226,227], allowing variables related with circularity and sustainability to be included from the start ("sustainability by design" [238]).
- The creation and, crucially, population with data of a modern, user-friendly, flexible, efficient, protected and especially attractive nuclear materials database, coupled with the consensual definition of materials examination protocols and relevant data format, is largely a prerequisite for the success of the above endeavours.

The concept of test bed, with different nuances of interpretation, is being applied to a large number of frameworks and technologies. In the case of healthcare, a test bed is a real life study, on a portion of population located in a specific region, of the effect of introducing innovative procedures, generally digitally-based, for the treatment of specific types of illness or patient condition. The study concerns all levels, i.e., not only or not necessarily the effects of specific drugs, but more importantly also how in practice the patients are treated with them and their conditions followed to check improvements. The UK National Health Service launched an interesting initiative of this type already several years ago [239]. In 2020 a similar initiative has been proposed, also in the UK, to test the implementation of innovative technologies related with climate change mitigation and adaptation, circular economy, clean energy, etc. [240]. In the case of advanced materials the EU supports test beds, in the sense described in Section 3.1, focused on nanotechnologies and functional materials [158]. Test-beds can be equally useful for nuclear materials, provided that there is willingness to integrate facilities, infrastructures and assets in general, which are spread all over Europe, under a single umbrella of coordinated, flexible and advanced exploitation. The spectrum of potential customers increases significantly if the test-bed is dedicated in general to materials operating under harsh conditions, of which irradiation is only one of many agents. A test-bed of wide application can be built incrementally, starting from pilot experiences that have limited targets and involve a limited number of participants, and then progressively moving towards higher levels of integration and flexibility. These small pilots will enable higher quality services to be provided to stake-holders for specific types of materials characterization, at a level that no single laboratory, and perhaps not even a single country, is generally capable of doing. It corresponds to institutionalizing what is customarily done in a collaborative research project for its limited duration, where the same material is characterised by different laboratories, each using the technique in which it is specialised or for which it can offer established, and perhaps unique, expertise. The combination of the results and their implementation in suitable models, e.g., of hybrid type, is the added high value of this collaboration, which, in the case of a test-bed, becomes stable. In addition, specific attention should be given to identifying, developing and standardizing accelerated non-destructive characterization methods, taking advantage of the possibility of using multiple techniques or multi-parameter hybrid techniques in a coordinated way and fusing their results, following protocols or designs of experiments that still need to be firmly established and, quite obviously, with the support of dedicated models. One significant issue when fusing results from different techniques is the use of a unique data format in order to be able to merge all these data in a common database. Harmonised approaches based on lessons learned when different laboratories apply the same physical principles of a method, using different ways of processing signals and data, need to be agreed upon. The technological challenge of creating a nuclear test-bed is significant, but it also has an important political and managerial dimension, which must not be underestimated.

Concerning modelling, Europe has a long, well-rooted and established history of projects dedicated to predicting the behaviour of nuclear materials in operation, especially under irradiation [165]. These projects have produced tools, skills and expertise especially in the framework of multiscale modelling approaches. These tools, skills and expertise need to be exploited at their best by blending them with emerging data-driven approaches, taking into account the specificities of nuclear materials issues. Among them, the most burning one is the almost chronic lack of sufficient data for model validation/calibration, as well as for qualification. While this can be partially offset by suitably integrated dedicated test-beds, hybrid models are expected to enable complex problems, for which purely physics-based modelling tools are still lacking (e.g., corrosion issues), to be addressed in a more effective way, so as to become usable for assessments also at industrial level. The challenge is here mainly theoretical and technical and will require the coordinated involvement of scientists of all ages, with a wide spectrum of expertise, providing the opportunity for young researchers coming from non-nuclear fields (e.g., digital techniques) to become involved in nuclear materials, and nuclear energy, applications.

The development of MAPs is exceptionally challenging in the case of nuclear materials, because of the complexity of the combined exposure, often under load, to irradiation, temperature and chemicals (fluids), with the subsequent difficulty of integrating the rapid and iterative evaluation of these effects on a single automated platform, using indicators of long-term degradation resistance that are far from obvious to identify. Modelling and digital techniques are clearly of crucial importance here, as well, and here, too, advances can be made incrementally, by focusing on specific problems or techniques and then progressively integrating different aspects. While the goal may appear science-fictional, it is nevertheless essential that nuclear materials scientists do not lag behind and strive to make use of these new methodologies, adapting them to their specific needs, because no-one else will do this for them. The potential benefits that these emerging materials science approaches may bring are tremendous in terms of reducing costs and times towards the much needed nuclear innovation. The development of a "nuclear MAP", similarly to the "nuclear materials test-beds", is a challenge that only close collaboration at European level may have the chance of tackling. Like in the case of test-beds, such MAPs, dedicated to materials for harsh operating conditions, may also serve other energy technologies and would maintain the long tradition of nuclear applications to be the crucible for materials of wider application than just nuclear [241–245].

Finally, producing a centralised nuclear materials database sounds like a sort of utopia, because of the formidable challenges that this goal raises also from the legal and political points of view. It is, however, a clear and undeniable need, to which effort has been already and is still being dedicated [234,246]. The brief description of the related issues in

Section 3.5 hints at the fact that many of the related challenges can be addressed with the help of suitable digital tools and, especially, with the skill of database masters that should make its use fully fit for the purpose according to requirements, having the data providers and the data users' needs as the main criteria for the design of the database.

5. Conclusions

The number of possible nuclear reactor systems and nuclear energy policy strategies is finite, but fairly large, and almost all of them are being considered in Europe. Privileging one over another is largely a matter of political choice of a country, or strategic choice of a company, that the nuclear materials science community in Europe and elsewhere cannot make and cannot formally interfere with. This community, however, is called to stably provide the tools, skills and knowledge that should enable safer and more sustainable (in a broad sense) operation and construction of current generation reactors, as well as reduction of costs and time for design, licensing and construction of any next generation nuclear system, in the interest of, *a priori*, any country or customer company, and chiefly society. Likewise, although the classes of materials that are suitable for application in the nuclear energy field are limited, the possible choices of actual materials and combinations thereof cover a wide spectrum, especially for next generation systems. The definition of a programme of full qualification of a given material solution for a specific application and design is clearly the task of the organization, or consortium of organizations, that lead the specific project and should bear the relevant costs. However, once again the nuclear materials science community should stably provide the tools, skills and knowledge to explore the different possibilities and come up with a series of good materials solution candidates, with sufficiently good properties to justify (and enable) industrial production, out of which the designers of a specific system can make a choice based on their specific needs and move towards full qualification. Ideally, the proposed material solutions should be designed to respond to requirements, taking into account, as much as possible, also criteria that go beyond the strict engineering performance, i.e., including aspects of circularity and sustainability at large. The community should also guarantee the skills and knowledge for the full qualification, using at best available infrastructures and facilities.

Consistently, a European strategic research agenda in support of innovation and coherent with the goals of the Green Deal [247], in connection with the clean energy transition, needs to aim at developing and establishing ambitious assets that are specific in nature, but also of broad interest for a large spectrum of (nuclear and non-nuclear as well) industrial applications. Several European countries need to share this same goal, which should inherently allow all of them to valorise their own research assets, in terms of facilities and infrastructures, as well as knowledge and skills. It is here proposed that these goals can be the development and establishment of structured materials qualification test-beds and materials acceleration platforms for nuclear materials (or materials that operate under harsh conditions at large), as well as the development of multi-parameter-based approaches for materials health monitoring using different NDE&T techniques. Hybrid models that suitably combine physics-based and data-driven approaches can valuably support these developments, together with the creation and population of a centralised, "smart" database for nuclear materials, which should eventually become a reference for all classes of quality data, including from MTRs and surveillance or monitoring.

Annex 1—GenIV Prototypes and Demonstrators in Europe

Over the last couple of decades Europe concentrated on four industrial GenIV fast reactor prototype/demonstrator projects, namely: ASTRID [248], ALFRED [249,250], ALLEGRO [251] and MYRRHA [29,252], all of them promoted by the European Sustainable Nuclear Industrial Initiative (ESNII—see Annex 2). The first three are, respectively, the sodium, lead and gas cooled GenIV fast reactor demonstrators. The last one is a sub-critical lead-bismuth cooled reactor to be made critical through a proton accelerator and spallation reactions that produce neutrons (accelerator driven system—ADS [28,29,47]). The

ASTRID project, which was driven by French EDF, AREVA and CEA, has been recently (2019) cancelled [253]. The construction of the gas fast reactor demonstrator, ALLEGRO, that is being designed by the V4G4 Consortium [254], is more and more pushed towards the future. The lead-cooled fast reactor demonstrator/prototype, ALFRED, promoted by the Falcon Consortium [255], remains on track. Finally, the construction of MYRRHA has been partly enabled by the funding granted by the Belgian government to SCK CEN until 2038. However, MYRRHA is not thought as a power reactor, but rather as an experimental facility that can be used for several purposes, which makes use of, or anticipates, GenIV technology. In parallel, a spin-off company of KTH in Sweden, LeadCold, is working at the design of a lead-cooled SMR [256]. Concerning other GenIV reactor concepts, i.e., the supercritical water reactor (SCWR) and the molten salt reactor (MSR), work is underway in several European countries, although no structured industrial initiative has yet been created around any of them in Europe, e.g., within ESNII. The MSR is currently receiving close attention at research level, especially in France and in the Netherlands [257], as well as in the Czech Republic [258]. In parallel, two startups based in Denmark are promoting molten-salt-cooled SMRs for various purposes and with varying detailed features [259,260]. Finally, the HTR is the focus of the NC2I pillar of SNETP [261] (see Annex 2).

Annex 2—Nuclear Systems and Materials Dedicated Platforms in Europe

The Joint Programme on Nuclear Materials, JPNM [262], is, since 2010, one of the currently 18 joint programmes (JPs) of the European Energy Research Alliance, EERA, which altogether cover the full spectrum of low-carbon energy technologies and systems [263]. EERA was created in 2008 in support of the European Strategic Energy Technology (SET) Plan [264], which had been launched in 2007. EERA promotes cooperation among almost 250 (in 2021) public research organisations, under the motto "catalysing European energy research for a climate-neutral society by 2050", and by focusing on low Technology Readiness Levels (TRL < 5 [221]), i.e., mainly dealing with research towards innovation. In contrast, industrial implementation (TRL > 5) characterises the technology platforms and the industrial initiatives, which are described in what follows in the case of nuclear energy.

The Sustainable Nuclear Energy Technology Platform (SNETP), launched in 2007, supports and promotes safe, reliable and efficient operation of Gen-II, III and IV civil nuclear systems [265]. In May 2019, SNETP became an international non-profit association under Belgian law. It is considered by the European Commission as a European Technology and Innovation Platform (ETIP). Its members include industrial actors, research and development organisations, academia, technical and safety organisations, SMEs and non-governmental bodies. It stands on three pillars:

- NUGENIA (Nuclear GenII&III Alliance) [266]: It supports the R&D of nuclear fission technologies, with a focus on Gen II & III nuclear power plants, providing scientific and technical support to the community, through initiation and promotion of international R&D projects and programmes.
- ESNII (European Sustainable Nuclear Industrial Initiative) [267]: It promotes Generation IV Fast Neutron Reactor technology demonstrators and supporting research infrastructures, fuel facilities and R&D work. Designing, licensing, constructing, commissioning and putting into operation demonstrators for new reactor technologies is thus the main goal of ESNII.
- NC2I (Nuclear Co-generation Industrial Initiative) [268]: It promotes the demonstration of low-carbon cogeneration of heat and electricity based on nuclear energy, as an innovative and competitive energy solution. Its target is the commissioning of a nuclear cogeneration prototype within 10 years, to serve several energy-intensive industries using this low-carbon energy technology.

Annex 3—Pathways to Nuclear Materials Improvement for Next Generation Reactors

Pathways to improve austenitic steels from the viewpoint of swelling and corrosion resistance (especially against heavy liquid metals) are being explored. Higher swelling resistance is pursued via microstructure stabilisation with selected alloying elements (for instance AIM1 and its bettered version AIM2) [269–271]. Enhanced corrosion resistance is sought for with corrosion barriers, either by implanting aluminum to change the surface composition and induce the formation of a protective alumina layer [272,273], or by directly depositing alumina (or other ceramics) layers to coat the metallic substrate [274–276]. Alternatively, aluminum is added to the alloy composition, to enable the formation of a protective alumina layer that self-heals through contact with the oxygen that is contained in the circulating fluids, so-called alumina forming austenitic (AFA) steels [277–281].

F/M steels (e.g., T91, EM10, HT9, or reduced activation F/M for fusion such as EUROFER and F82H) outperform austenitic steels by offering higher thermal conductivity, lower expansion coefficient and, especially, remarkable resistance to radiation-induced void swelling [79,88], thereby revealing themselves as very suitable cladding and core materials. For fusion applications F/M steels are essentially the only possible choice, because they offer the possibility of tuning their composition to reduce significantly their end-of-life activation: no other class of steels suitable for nuclear applications offers this possibility. In GenIV applications swelling resistance is key to reaching high burnups by attaining 200 dpa (or more) in the cladding. However, F/M steels can currently operate only below 550 °C [79,88,282,283], because of insufficient creep resistance. They also suffer from significant radiation-induced embrittlement below 350–400 °C [79,88,284–286] and are especially prone to liquid metal embrittlement (LME) when in intimate contact (wetting) with heavy liquid metals (HLM), i.e., Pb-based alloys [287–289]. Reliable correlations and models for the identification of design rules are therefore needed for this class of materials. Work in this direction is being done in the case of EUROFER, the 9%Cr reduced activation F/M steel that is envisaged as main structural material in the European fusion DEMO [290–292]. However, the compatibility with HLM and the resistance to high temperature and embrittlement of F/M steels need to be improved, in order to reach higher levels of efficiency and better economy. Two pathways are pursued to improve the creep properties of F/M steels: (1) use of oxide-dispersion strengthened (ODS) steels [93,293–297], with a target of 700 °C or beyond as upper limit operating temperature [93,293,294]; (2) composition-tuning and application of suitable thermal-mechanical treatments (TMT), in a conventional metallurgy framework, with a target upper temperature limit of 650 °C [294,298–301]. Metallurgical techniques of the second type may also help to control radiation embrittlement below 350 °C [302]. ODS are still manufactured using costly powder metallurgy techniques of difficult industrial upscaling, thus alternatives are being looked for [303–305]. Moreover, they offset creep resistance with still relatively poor fracture toughness and low temperature embrittlement [295,306]. However, they offer significantly improved radiation (swelling, helium embrittlement, . . .) resistance at high temperature [93,293,295]. Finally, the methods to improve F/M steel corrosion resistance are the same as in austenitic steels: either surface modifications/coatings [307–310] or alloy composition tuning with aluminum addition, so-called FeCrAl (currently intensively studied for ATF cladding) [311–315]. The latter may also be ODS, giving rise to a potentially very promising material (ODS-FeCrAl) that is simultaneously resistant to irradiation, creep and corrosion [316–318].

For temperatures close to, or above, 800 °C, no known steel can maintain its fitness for purpose, with the partial exception of high Ni austenitic steels such as alloy 800 [95], which are therefore considered in GFR and (V)HTR. Ni-based alloys (e.g., Inconel 617, Haynes 230 and Hastelloy XR) are in this case possible candidates for components outside the core, particularly heat exchangers [90]. However, under irradiation these alloys suffer from quite severe irradiation embrittlement and also swelling, due to helium production by transmutation from Ni [89,319–321], so their use in the core may be critical. Yet, because of high temperature compatibility issues, these alloys are likely to be the only possibility as core materials in the case of MSR prototypes [322–325]. One possibility to use these alloy as reactor core materials could be the development of ODS Ni-based alloys, as the oxide dispersion would produce traps for helium and improve radiation resistance [326–328], like in the case of F/M ODS steels. Otherwise, refractory elements need to be considered for in-core applications, including ATF. The spectrum of alloys is quite wide [96,97,329], for both fission and fusion [330] and especially considered for space nuclear applications [331], often combining elements, either in solid solution [96,97,329], or in layers [332,333]: molybdenum alloys [102,334,335] (U-Mo alloys are also considered as proliferation-resistant fuel [336].), niobium alloys [331,337], vanadium alloys [97,333,338–340] and tungsten alloys [332,341,342], the two latter especially for fusion, and tungsten exclusively for it [329,342]. Tantalum alloys have been considered in the past in the US for space nuclear applications, but little information is available, except for a few conference abstracts that can be found online. The main problem with refractory metallic alloys is their brittleness, so generally developmental efforts are aimed at alleviating this feature. Moreover, as in the case of F/M steels, both for Ni-based and even more for refractory metallic alloys, suitable design rules need to be established.

Beyond refractory metallic alloys, ceramics generally offer very attractive properties in terms of both stability to high temperature and resistance against wear and corrosion/erosion [343], the most commonly studied being SiC_f/SiC (i.e., silicon carbide fibres in silicon carbide matrix) composites [90,98–100,344], C_f/C (carbon fibers in carbon matrix) composites [345] and alumina nanoceramics (mainly as protective coating) [346]. Not by chance is nuclear fuel currently used in the form of a ceramic (UO_2, PuO_2, . . .) [106–108], as well. However, when used for structural purposes, these materials are penalised by significant brittleness. This is why refractory materials for structural components, not only ceramics as above, but also metallic [335,341], are generally considered in the form of composites, containing fibres or other reinforcements that provide some type of pseudo-ductile mechanical behaviour. Other possibilities may be layered materials [332,333,347], or nanocomposites [101,347].

SiC_f/SiC is the main candidate material for GFR cladding [90,344]. It is also a material of use for the (V)HTR [98,99], in addition to the more conventional graphite [62,91,348], and it is in principle also a suitable candidate ATF cladding [99], as well as for LFR and SFR, in order to safely reach higher temperature and dose than with metallic cladding. However, this material remains at low TRL and quite expensive to fabricate [99]. Furthermore, as for essentially all ceramics that are considered for structural functions, design rules for it are not developed [90].

The design of the high temperature gas cooled reactor concepts (GFR, V/HTR) also requires appropriate materials solutions for thermal shielding and insulation, fuel matrix, neutron reflectors and suitable control rods and seals, that would be operating close to 1000 °C, or above and up to 1650 °C in accidental scenarios [90,349] These materials must guarantee at those temperatures properties of gas-tightness and corrosion resistance, with the ability to be joined. At the moment, in addition to SiC, other materials such as C_f/C, mullite (aluminosilicate), Al_2O_3, TiO_2, ZrC, ZrN, Zr_xSi_y, B_4C, WC, graphite or even graphene are being explored for these functions [90,349–352].

Further gateways to improved future reactor performance are opened by perspective, generally ceramic or metallic refractory, materials, with specific radiation resistance features [101,347]. Examples range from ODS-Mo alloys [102] and the already mentioned layered materials [332,333,347] or nanocomposites [101,347], to high entropy alloys (HEA) [103,353–355], or the wider class of complex concentrated alloys/compositionally complex alloys (CCA) [104,356,357], and MAX phases [105,358–362]. These are classes of materials of still very low TRL, which, however, do appear to be promising in terms of corrosion and radiation resistance, especially HEA/CCA [103,363–367]. These may have applications as cladding materials [368,369], or to devise especially radiation resistant refractory alloys for fusion applications [370–372]. CCA, characterised by being alloys with many elements, none of which is dominating, and perhaps partially also MAX phases, raise especially high interest because of the possibility of applying to them the combinatorial methods of fabrication. This feature is very suitable to apply modern techniques of autonomous materials discovery and development that are put forward in this paper, which are based on the integrated use of high throughput automated characterization and data-driven modelling, with the support of artificial intelligence [225].

An interesting overview on European Commission research on GenIV safety and materials is provided in [373].

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