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European Materials Development: Results and Perspective

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This paper addresses the EUROfusion DEMO materials research program and highlights the characterization of the in-vessel baseline materials EUROFER97, CuCrZr and tungsten as well as advanced structural and high heat flux materials developed for risk mitigation. In support of engineering design activities the focus primarily is to assemble a data base, to supply material property handbooks, material assessment reports, DEMO design criteria and material design limits for DEMO thermal, mechanical and environmental conditions.

For advanced candidate material including (a) steels optimized towards lower or higher operational windows, (b) heat sink materials (copper alloys or composites) and (c) tungsten based plasma facing materials data representative for DEMO are presented.

In view of preparing for future licensing and clarification of performance limits, as major step nine neutron irradiation campaigns were started recently. The campaigns include (i) baseline materials irradiated up to medium neutron dose levels, typical for DEMO 1st phase, to fill gaps in the materials property handbook and improve design limits (ii) advanced material irradiated at lower fluence for screening and down-selection and (iii) a huge temperature-dpa matrix at low fluence for material modelling verification and increased fundamental knowledge.

Keywords: RAFM-steels, tungsten and copper based composites, DEMO design criteria, neutron irradiation

1. Introduction

DEMO and future fusion power plants will need robust materials incorporated into reliable components for the inner vessel (blanket and divertor), able to perform best and safe under the combined neutron, thermal and mechanical loads. The list of requirements including heat removal capability, neutron and gamma shielding, tritium production and inventory, extended lifetime, easy industrial manufacturing and restrictions, in particular activation and waste, narrows down chemical composition and material classes significantly and has led to a reduced, but still quite extensive portfolio.

A specific fusion challenge is that in addition to the neutron induced displacement damage observed with fission neutron spectra as well, the high energy neutrons in a fusion spectrum produce He and H in components near to the plasma with generation rates that can be orders of magnitude higher than in fission based Material Test Reactors (MTRs). This shall substantially accelerate irradiation embrittlement, depending on (irradiation) temperature and deformation rate, and may promote early degradation and failure.

Based on material developments and assessments performed in the frame of EFDA [1-4] the main objectives for blanket and divertor related material development within the EUROfusion Workpackage Materials (WPMAT) from 2014 until the beginning of the engineering and design phase for DEMO foreseen in 2027 include: (a) to characterize and to finally validate baseline materials, (b) to develop “advanced” materials for both, risk mitigation and selectively improved properties, and

(c) to develop an adequate engineering materials property handbook and design criteria for DEMO operational and environmental conditions.

The portfolio of baseline structural and high heat flux materials comprises the structural and armor baseline materials for DEMO: (i) EUROFER(97), a 9Cr RAFM (Reduced Activation Ferritic Martensitic) steel, as structural material for the breeding blanket, (ii) tungsten as plasma facing component armor material, and (iii) CuCrZr as heat sink material for the divertor coolant interface.

The advanced structural and high heat flux materials are presently assumed to be of the same material class as the portfolio of baseline materials, i.e. RAFM steels and tungsten, and copper alloys or composites. The development of advanced steels focuses on 9Cr RAFM to be optimized for operation at (a) lower temperature together with water-cooled breeder blankets (BB) application (b) higher temperature helium cooled BB options aiming for higher thermal efficiency, and (c) on fabrication of higher Cr ODS (oxide-dispersion strengthened) steel options. Similarly, advanced materials for high heat flux applications have to be developed, which include fiber- or particle-reinforced materials. Attention must also be paid to scalability in manufacturing towards industrialization.

The strategy for design and licensing of divertor and blanket structures is driven by material performance limits and constraints in knowledge. It is foreseen that DEMO will utilize a starter blanket using EUROFER RAFM steel and conservative design margins with a restricted

operation window where He-effects are considered minor to moderate. For water cooled blankets using RAFM steels, and limited by the low temperature end of the window, two full power DEMO years corresponding to the generation of 20 dpa neutron damage (displacements per atom) is considered as safe operation. A period of operation with a second set of blankets aims for longer life (equivalent to ~ 50 dpa). The challenge for the next decade is the development of materials technology including various options for joints (and their proper and full qualification under irradiation), barriers and coatings.

Currently, the engineering material data, both properties as well as verification and further development of design rules, are based on still scarce fission neutron irradiation campaigns, not covering the full temperature window nor the complexity of environmental and loading conditions (e.g. periodic, gradients, multi-axial). Therefore, large uncertainties have to be compensated in engineering design by large and likely too conservative, safety factors. The demand for improved design criteria is the driving force for obtaining additional and more data and an improved knowledge on operation limits and damage/failure modes. Achieving all this needs various and comprehensive irradiation campaigns in MTRs as soon as possible, complementary experiments with multi-ion beam facilities, as well as a range of complementary materials test facilities including high heat flux and plasmas. Data gathered and information shall be tied together with a comprehensive multi-scale modelling program with mandatorily high predictive capability and, in a wider frame, with multi-physics modelling tools to be developed and applied in the interface with (in-vessel-component) engineers. The final validation and qualification of materials and design rules for DEMO operation, in particular for safety reports to be submitted to licensing and regulatory authorities, imply additional requirements such as experiments under neutron spectra typical for fusion (plasma near) conditions. A powerful dedicated (14 MeV) fusion material neutron source (FNS) is mandatory and needs to be as well available as soon as possible. Facilities fulfilling the (reduced) scope of material property validation for early DEMO operation are under discussion and preparation to be built in Europe, called DONES Europe [5] and in Japan, called A-FNS in Japan [6], where both facilities have the capability to be upgraded and scaled towards the “full” IFMIF [7], the FNS planned and developed under the umbrella of IEA in the past and EU-JP Broader Approach since 2008.

2. Materials development program

DEMO requires the development of structural materials for inner vessel components, in particular the breeding blanket, withstanding neutron damage of targeted 50 dpa in the operational temperature regime. Furthermore, (improved) divertor materials, are needed that can withstand combined high steady state and transient heat fluxes under low to moderate neutron loading (e.g. 4-8 dpa for tungsten and 10-20 dpa for copper based materials). Materials development qualification and validation, as indicated by similar

challenges as from fission or Apollo is expansive [8] and has lead times of approximately two decades. Whilst final validation of the materials for DEMO as a nuclear facility with unprecedented loading and damage scenarios will be strongly dependent on the availability of a fusion representative facility like IFMIF, substantial advances on this long path have been made in the field of materials development and qualification as well as damage modelling.

2.1 Advanced steels

Design windows for materials like EUROFER97 are multi-faceted in a multi-dimensional design space and have to be determined for each design concept individually. Reducing it to the variable “operational temperature”, the area of safe operation even in excess of 20 dpa and 500 appm He content is ~ 350 - 550°C , determined by neutron induced embrittlement at low temperatures (neutron damages and He-transmutation) and softening at high temperatures. Performance limits likely can be extended towards 300°C , however cannot be guaranteed from today’s experimental database, as the brittle to ductile transition (BDT) temperature is strongly sensitive to the helium content (formed by neutron induced transmutation) with a steep gradient at a certain threshold concentration. This is a prominent example where the final answer has to be provided by a FNS (IFMIF).

Steel developments focus on improvements of 8-9% Cr RAFM steels for two operational scenarios: (i) water cooling with the emphasis on good low temperature performance starting from coolant temperature ($\geq \sim 300^\circ\text{C}$ [9]); (ii) helium cooling with the emphasis on improved high temperature performance to extend the operational temperature regime towards 650°C . In both cases the properties at the respective other end of the temperature window should be kept as much as possible.

In parallel, developments on the fabrication towards industrialization of 9 and 14% Cr ODS-steels via standard and novel methods are ongoing. These materials in the time frame of DEMO likely are candidate only first wall (FW) design options (such as plating a “separated” FW) however are a very promising candidate for commercial nuclear fusion power plants due to their nanostructure that indicates improved neutron resistance and high temperature application for high thermal plant efficiency.

2.2 High heat flux materials

This class of materials consists of plasma facing materials for the divertor and the breeding blanket, heat sink materials to be used in the divertor region and interfaces between these materials as well as joints. The latter are aiming for creating components with an improved structural stability under the operational thermal and neutron loads with a sufficiently high heat removal capability.

Plasma facing materials have seen a long-term development in Europe with the focus on W-based materials that has now concentrated in particular on particle and fiber reinforced composites as well as the combination of highly ductile tungsten sheets to a tungsten laminate. The reinforcement by particles, e.g. TiC and Y₂O₃, and fibers, i.e. W and SiC, as well as the laminates are tackling the issues of intrinsic low temperature brittleness, neutron induced embrittlement and recrystallization resistance of tungsten. Neutron embrittlement in pure tungsten occurs up to temperatures of at least 600-800°C strongly limiting the low temperature operational range while recrystallization occurring between 800-1500°C depending amongst others on the deformation history of the material and its impurity level provides the upper limit (typical value for ITER grade tungsten: 1300°C). Furthermore, in view of accidental scenarios including a loss of cooling combined with water and/or air ingress, self-passivating tungsten alloys primarily for the first wall of the breeding blanket but also for areas in the divertor with reduced power handling needs are developed to avoid extensive erosion of tungsten by the formation of volatile radioactive tungsten-oxide.

Heat sink materials for the divertor comprise materials suitable for water cooling applications (actually foreseen coolant temperature ~150°C) with comparably high thermal conductivity, i.e. particle and fiber reinforced Cu-based materials. The high thermal conductivity is essential to allow components with a heat removal capability of up to 20 MW/m² under steady state heat loads. Similar to EUROFER97 the design window for CuCrZr needs to be determined for each design concept individually. Accordingly, operation in water cooled divertor concepts at ~150°C might be feasible, however, due to neutron embrittlement and in particular the loss of uniform elongation at temperatures below ~200°C and neutron softening above ~300°C this would be the recommended temperature range for safe operation [10]. Therefore, developments of tungsten particle and fiber reinforced CuCrZr aim at increasing this range to the lower as well as the upper side. The latter is important to close the operational temperature gap to the plasma facing material.

Alternatives to reduce this gap are tungsten laminates using highly deformed and therefore ductile tungsten sheets in combination with other ductile materials (Cu, Ti, V), which may be used as heat sink or, alternatively, as interlayer materials. Other potential interlayers are W/Cu functionally graded materials (FGMs) and thermal barrier materials or structures which allow, if used only at high heat flux side of the component, achieving a more homogeneous temperature distribution within the high heat flux component.

2.3 Engineering data and design integration

For the qualification of materials and their implementation into the design, establishing a functioning materials design interface is crucial. First steps in this direction are the development of a reliable material

database for baseline and advanced materials and the compilation of a (DEMO) Material Property Handbook. The handbook should contain information on all design relevant material properties for all baseline materials and those advanced materials that have achieved a sufficiently high materials technical readiness level (MTRL) and proven to be a viable alternative.

Besides material properties, nuclear licensing of a facility like DEMO requires the development of design rules to be compiled as DEMO design criteria (DDC). This comprises on the one hand the adaption and re-writing of existing rules from existing design criteria and codes like RCC-MRx and ITER-SDC and on the other hand the development of new rules for specific and unique loading cases for nuclear fusion facilities. This is mainly but not only due to the high-energy neutron loading and addresses in particular the highly loaded inner vessel components.

Both, the development of the material property handbook and the design rules require an extensive amount of materials testing for determining design allowables and validation of rules in the non-irradiated and irradiated state.

2.4 Irradiation and irradiation modelling

Neutron irradiation is an indispensable tool not only for the determination of material properties but also for the qualification of newly developed materials. Test campaigns in material test reactors (MTRs) were launched on baseline (EUROFER97: 20 dpa; tungsten: 1 dpa; CuCrZr: 5 dpa) and advanced materials (up to 1 dpa in tungsten) (i) to obtain design relevant engineering as well as modelling data for the baseline materials and (ii) to allow a qualification of improvement and reinforcement strategies for advanced material concepts.

Multiscale modelling is a tool now widely used in industry to simulate complex processes, and design engineering structures, including cars and aircrafts. This has not yet been fully exploited in the context of fusion, largely because the models for irradiation effects developed so far were not compatible with finite element modelling analysis. This barrier has now been overcome through the development of a treatment combining cascade simulation data, large-scale density functional theory calculations, million-atoms cell atomistic simulations, theory of elasticity and finite element modelling [11] enabling extensive application of multiscale modelling simulations to the assessment of fusion power plant design options. This highlights the growing predictive capability of computer simulations, providing new means for the assessment of materials lifetime and fusion power plant design options.

3. Materials R&D highlights and conclusions

3.1 Advanced steels

In a first step, 30 new alloys, specified since 2014 as either EUROFER-LT (low temperature) or EUROFER-

HT (high temperature), were successfully cast and microstructural and mechanical characterization has been completed that allowed material down-selection for further qualification via neutron irradiation. Based on these first results, additional alloys were designed and manufactured in 2016 and characterization of these materials is ongoing.

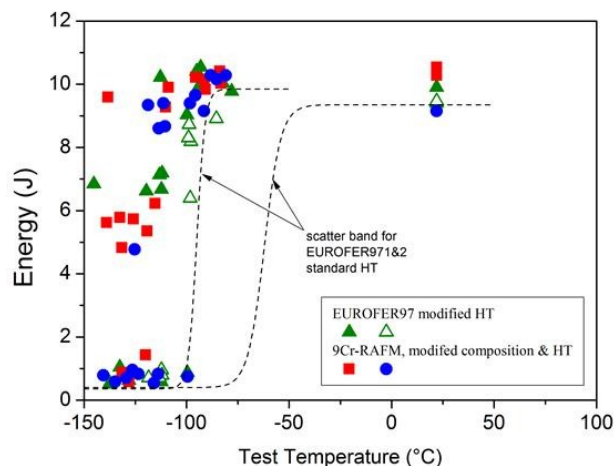


Fig 1: Charpy impact test data (KLST) for optimized RAFM steels in comparison to EUROFER97 1&2 and standard heat treatment (HT)

The development of 9Cr steels for LT application is a challenging objective, since EUROFER97 in its standard metallurgical condition is already an optimized steel in terms of impact and toughness properties with a BDT in a scatter band from $\sim 100^{\circ}\text{C}$ to -60°C . Furthermore, it exhibits much better irradiation performance at low temperature than conventional 9Cr FM steels [12]. However, with optimizations of the material composition and the use of thermal and mechanical treatments some improvement of impact properties in the as-manufactured condition, i.e. a reduction of the BDT to $\sim 120^{\circ}\text{C}$ has been obtained (Fig. 1). As the probability that further optimizations of the chemical composition and the application of new treatments may yield more significant gains is low, the focus and material manufacturing has shifted towards the investigation of new alloy compositions and microstructures aiming at reducing irradiation-induced hardening and embrittlement, in particular in view of fast neutron induced He-embrittlement.

The results for EUROFER-HT show that the development of 9Cr steels for HT applications is a realistic goal. For instance, high temperature creep and fatigue properties were significantly improved (Fig. 2) by using simple, non-standard heat treatments. By the optimization of the chemical composition as well as the use of special heat treatments and thermo-mechanical treatment conditions further improvements were obtained that resulted in the increase of the upper limit of the operational temperature range of EUROFER by 50-70 K [13]. Further optimization and combination of composition and thermo-mechanical treatments are ongoing with the actual goal to increase the upper limit towards 650°C without degradation of impact/toughness properties on the low temperature side.

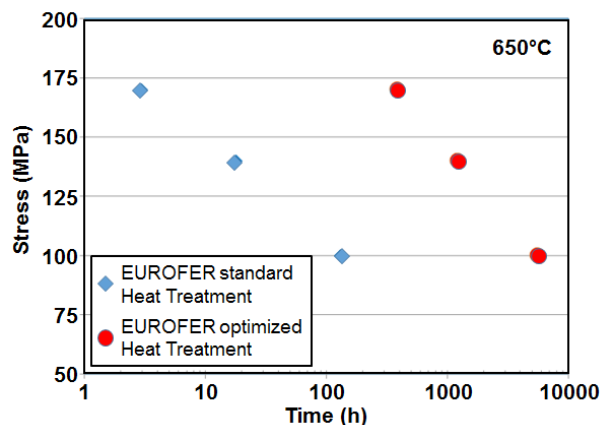


Fig 2: Creep lifetime (time to rupture) for EUROFER in the standard metallurgical condition and after non-standard, optimized heat treatments at $T = 650^{\circ}\text{C}$

One important goal in the fabrication of ODS-steels, i.e. the “large” scale fabrication, has been achieved by fabricating a batch of 30 kg of 14Cr-ODS steel using the standard fabrication route of mechanical alloying, sintering and subsequent hot and cold rolling to obtain large plates with a thickness of 2-3 mm in the range of square meters. These plates are one potential alternative for the structural parts in plasma facing units already in DEMO that are closest to the plasma and therefore experience the highest temperature and neutron loads. Accordingly, a First Wall mock-up with ODS plating has been fabricated and is ready to be tested in the high heat flux test facility at KIT using He-coolant.

In view of a future fusion power plant, further developments of ODS materials would require the manufacturing of even larger/thicker material pieces in order to allow replacing EUROFER for the whole plasma facing unit by the ODS-steel. This goal is tackled on the one hand by further exploring standard processes and on the other hand by exploring the ODS production using alternative routes. These routes try to avoid the comparably time and cost intensive powder production using mechanical alloying by atomization processes and reaction synthesis [14]. Significant advances were achieved by the successful production at industrial scale of high quality powders containing Y and Ti, which is a major step forward towards industrial fabrication. However, this is only the prerequisite and similar to the standard fabrication route now the mechanical strength of ODS produced with the new route needs to be improved. Thereby, further optimization and modification of the process with implementation of hot deformation is an actually followed promising approach.

3.2 High heat flux materials

3.2.1 Plasma facing materials

Since 2014, more than 30 new tungsten materials and composites (pure W and additions in the range of 0.5 – 8wt.% of W_2C as well as TiC, TaC, La_2O_3 , Y_2O_3 , HfC, HfO, Re and combinations thereof) were produced via various sintering techniques and powder injection molding

(PIM) [15], a near net-shape and also mass-fabrication technology, for screening and benchmarking towards industrially produced tungsten materials via ELM-like transient high heat flux testing [16]. Thereby, particle size and distribution are essential quality criteria and in particular carbide containing materials have shown in high heat flux tests the potential to outperform industrially produced tungsten materials. First mock-ups using the ITER design and containing pure W materials produced via PIM have been manufactured and high heat flux tested up to 1000 cycles at 20 MW/m² (Fig. 3). The manufacturing and testing of mock-ups using selected advanced tungsten composites is actually ongoing.

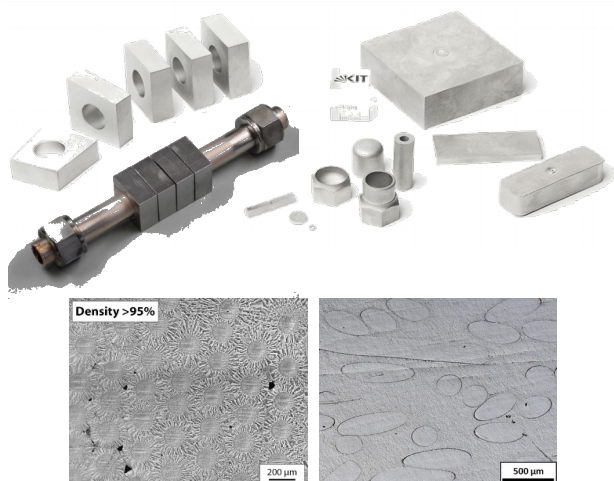


Fig 3: Various tungsten pieces produced via PIM and the produced mock-up after exposure to 20 MW/m² (top); microstructure of long and short fiber reinforced tungsten (bottom)

Tungsten-fiber reinforced tungsten composites were developed in two variants, (i) long fiber reinforced composites produced via chemical vapor deposition (CVD, Fig. 3, left) and (ii) short fiber reinforced composites (Fig. 3, right) produced via field assisted sintering techniques (FAST) in combination with a final densification via hot isostatic pressing (HIP) [17, 18]. In both cases, potassium doped tungsten fibers were used to take benefit of their high temperature stability/recrystallization resistance and both options show a pseudo-ductile behavior, i.e. even in the brittle regime no catastrophic brittle failure occurs. Thereby, the combination of fiber, matrix and novel developed interfaces like Y₂O₃ is decisive to take benefit of processes like crack deflection at fibers and fiber pull-out. The development of new devices for the upscaling of the material production and for a more economic material screening is ongoing.

Self-passivating tungsten alloys containing Cr as oxide forming element as well as an element that stabilizes the oxidation process (e.g. Ti, Y or Zr), which is controlled by element diffusion, have been successfully produced via mechanical alloying to obtain the required fine distribution of elements followed by HIP or spark plasma sintering (SPS) [19, 20]. The materials provide an increase of the oxidation resistance by up to a factor of 10⁶ in a temperature range up to 1000°C in dry and humid atmosphere. While still providing an increased brittleness

compared to the other developed tungsten composites, which is one of the next development issues, they have shown increasing mechanical stability and comparable resistance under transient thermal loads.

3.2.2 Heat sink materials

The most developed and already industrially available heat sink material for water cooled applications is tungsten particle reinforced Cu and CuCrZr [21]. Thereby, the preference is on CuCrZr in view of the swelling performance under neutron irradiation and it shows a significantly improved mechanical performance (strength, fracture toughness) and stability compared to CuCrZr in the non-irradiated state up to temperatures of 500-550°C (Fig. 4).

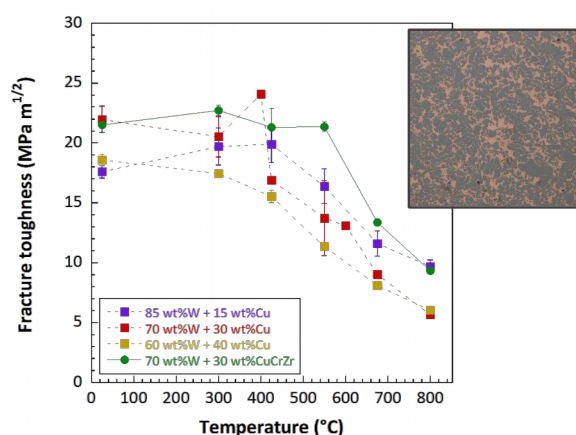


Fig 4: Fracture toughness of W-particle reinforced Cu and CuCrZr; microstructure of one of three industrially produced batches of W_p-CuCrZr

Similarly, W-fiber reinforced CuCrZr is developed in collaboration with industry and material in the shape of plates and tubes [17, 21]. These are produced using woven tungsten fiber fabrics that are subsequently liquid melt infiltrated and thermally treated. For both cases, ITER shaped mock-ups were produced, which survived high heat flux testing up to 500 cycles at 20 MW/m² without indication of failure.

For He-cooled applications, tungsten laminates are aiming for a ductilization of tungsten [22]. Laminates were produced in the form of plates and tubes using ductile tungsten foils with interlayers of Cu, CuCrZr, Ti and V. While all materials are showing ductile behavior at room temperature in the non-irradiated state, strong emphasis has to be put on the materials interface and the long term stability under operational conditions. Thereby, Ti and V are prone to react with tungsten and for the use of these materials, additional thin interlayers, e.g. Cr or Cu, are required.

3.2.3 Interfaces

Thin (~15 µm) and thick (~0.5 mm) W/Cu-FGMs were developed and produced via PVD and plasma spraying processes [23]. While mock-ups built according to the ITER-like monoblock design containing the thin FGM have been already fabricated and tested up to 1000 cycles at 20 MW/m², mock-up manufacturing using thick

FGMs, which are expected, according to finite element analyses, to result in an improved mitigation of thermal induced stresses, is actually ongoing.

For a very particular design option relying on a more homogeneous temperature distribution with the component, thermal barrier materials are developed using flexible amounts of oxide and carbide additions to Cu (e.g. SiC, ZrO₂, C) [24, 25]. These were fabricated using FAST and exhibited thermo-physical properties tunable over a wide range, i.e. from pure Cu at ~ 400 W/m.K down to a few W/m.K. The fabrication of suitable inserts into an optimized monoblock design based on FEM-analyses and implementation into mock-ups is actually performed and proof of principle should be done via high heat flux testing.

Independent on the use of the material as plasma facing, heat sink or interface material, it is decisive in all the manufacturing and testing processes containing tungsten to avoid carbon in the system. Diffusion of carbon and the uncontrolled formation of tungsten carbides results in a significant embrittlement of the material [26].

3.3 Engineering data and design integration

One of the key achievements to date is the establishment of a database that includes over 10,000 carefully assessed and collated individual records from literature, existing databases and from advanced material development [27]. This database is the source for the Material Properties Handbook (MPH) for which the second release of the EUROFER97 chapter represents the best available source of information of EUROFER97 despite the still existing substantial gaps due to a lack of irradiation modified data [28]. Further chapters on the baseline materials tungsten and CuCrZr are in preparation. However, in particular for tungsten a significant number of challenges were identified, including but not limited to unknown tungsten specification for the components, significant variability in properties between different tungsten production techniques and manufacturers and even batch to batch variability from the same manufacturer, unknown processes for tungsten manufacturing, unknown requirements of materials properties to validate the designs [3, 16, 29]. Due to a too large variability in the material properties it is not yet possible to provide the designers with acceptable materials allowables from this sparse dataset and the set-up of this chapter requires the clear definition of a baseline tungsten material in collaboration with industry.

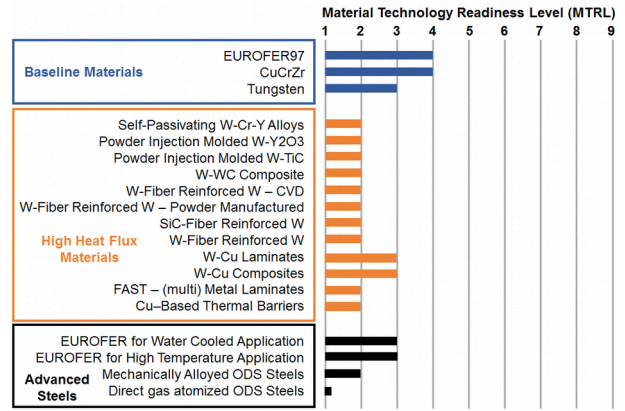


Fig 5: MTRL of baseline materials and advanced steels and high heat flux materials

Besides the baseline materials all other developed materials are characterized by rating them with a defined Material Technical Readiness Level (MTRL) from 1 to 9 with 9 being the highest level representing a well-established and used material for a certain application. While for the application in DEMO, a level of 7 would be required, the actual baseline materials are at level 4 (tungsten still at the verge from 3 to 4) and the newly developed advanced materials have yet achieved level 2 to 3 (Fig. 5).

In the frame of establishing the DEMO Design Criteria (DDC), for which material data (properties and limit data) are the main input, its structure consisting of General Information, Structural Integrity Assessment, Analysis Guidelines and Rule Justification has been produced, populated with selected draft content, and is now subject to ongoing industrial peer review [30]. For the part on design rules, development work is performed amongst others on ratcheting, fatigue, brittle fracture, multi-axial fatigue, exhaustion of ductility and creep-fatigue. Despite a lack of neutron irradiation data for the applied materials in particular at high irradiation dose and under a fusion neutron spectrum, design rules for ratcheting, exhaustion of ductility, fatigue and creep-fatigue have reached a point where guidance on these updated rules can be provided. In particular, the developed creep-fatigue tool has been rolled out to designers with peer reviewed feedback [31]. Nevertheless, further time and cost intensive rule validation testing for the above mentioned damage modes is required in the non-irradiated and irradiated state.

In addition, a strategy document for the materials design interface was developed. This includes a strategy for the future development of fusion specific design rules focusing on three primary assessment routes that can be applied, i.e., elastic analysis, in-elastic analysis, or multi-scale physics analysis depending on the requirements of the design [30]. Complementary to these deterministic approaches a probabilistic based assessment was considered viable and to be investigated [30].

Table 1. Neutron irradiation campaigns launched within EUROfusion WPMAT

Campaign	Material	dpa	T [°C]	Property	End of irradi.
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Blanket Baseline Design	EUROFER	20	200-350	Tensile, toughness, R-curves	Dec-2019
Divertor Baseline Heat Sink Design	CuCrZr	5	100-300	Tensile, toughness, LCF	Aug-2019
Tungsten Basics	W	1	400-1200	Toughness	Jun-2018
Validation Data for W Modelling	W	1	600-1200	Hardness, strength	Dec-2017
Screening of Advanced Steels	9% Cr steels	2.5	300	Tensile, toughness	Apr-2017
Screening of HHF Properties	W composites	1	600-1200	Thermal shock and plasma loading	Sep-2018
Screening of heat sink materials	Cu alloys / composites	1 (W)	150-450	Tensile	Mar-2019
Screening of plasma facing materials	W alloys / composites	1	600-1100	Bending, BDT	Mar-2019

3.4 Irradiation and irradiation modelling

In 2016 and 2017, eight irradiation campaigns were launched and their objectives and specifications as well as the expected end dates are given in Table 1. Four campaigns aiming at obtaining design relevant data for the baseline materials and the remaining four campaigns explore the improvement and reinforcement strategies for advanced material concepts. Results from post irradiation examination (PIE) are expected to be available, depending on the respective campaign, from 2018 to 2020. Further extensive neutron irradiation campaigns in MTRs will be required in the coming years accompanying the conceptual design phase for DEMO and addressing gaps in the material property handbook and design rule development.

In modelling radiation damage, a new algorithm, combining semi-empirical potentials and ab-initio based molecular dynamics, as well as a BCA-MD (binary collision approximation – molecular dynamics) model for more computationally efficient simulations exploring larger spatial scales via accelerated MD, were developed to obtain better and more reliable predictions for the initial populations of defects produced by irradiation [32]. Simulations also show a potentially significant effect of pre-existing defects (for example dislocation loops and vacancy clusters) on the accumulation of subsequent damage [33, 34]. This is a new and significant finding as radiation defects in engineering materials accumulate not in perfect crystal lattices, often explored in simulations, but in complex microstructures containing pre-existing defects, dislocations, grain boundaries and precipitates.

The relaxation and evolution of the damage produced by cascade events occurs at comparatively long timescales, often comparable with the interval of time between the subsequent cascade events, especially in the low dose rate limit. The models that are being explored here span the interval from stochastic kMC approaches [35] to diffusion-mediated dislocation based models [36] to rate theory cluster dynamics type simulations that are expected to be able to help explain the observed evolution of radiation induced microstructures [37].

The phase stability of alloys requires comparing the free energies of competing phases; new methods of analysis are being developed and validated for this purpose. Simulations of complex W-Re-Os show that radiation defects may act as centers for precipitation of Re and Os rich phases [38, 39]. In FeCr alloys, new models for segregation of Cr to grain boundaries show the

significant part played by the many-body hopping events, and also by the correlated motion of carbon, nitrogen and oxygen, substitutional impurities, and irradiation induced vacancies [40, 41]. Finally, the mechanisms responsible for the fracture of steel containing Cr-carbides were successfully simulated [42].

Dislocation based models are a major area where greater effort has been applied and even more is needed in the future. Results obtained so far already show that the observed jerky motion of dislocations can be explained by effects of heat spikes associated with the nucleation of double kinks [43]. There is still unresolved issue about the lack of formalism needed for including temperature effects in dislocation dynamics and plasticity simulations.

Microstructural evolution models that use the rates of defect production and temperature as input produce information about the local volume densities of defects at various locations in the structure [11]. The density of defect relaxation volumes provides a direct input to FEM calculations of temperature fields as well as stresses and strains in the reactor structure. The generation of irradiation induced stresses for tungsten in the vicinity of radiation induced defects is shown in Fig. 6.

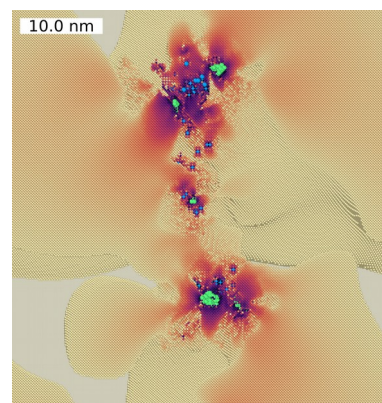


Fig. 6. A diagonal component of the stress tensor, plotted using a colour scheme reflecting the magnitude of stress, in the vicinity of radiation defects produced by a 150 keV neutron impact in pure tungsten. The green and blue spheres are the interstitial and vacancy defects, respectively, identified using the Wigner-Seitz cell analysis (image courtesy of A.E. Sand, [33]).

Also, the long-standing puzzle of radiation embrittlement (Fig. 7) has now been unraveled, showing that the origin of it is associated with the two-fold increase of the effective activation energy for migration of dislocations in steels or tungsten occurring in the limit where the volume density of radiation defects, acting as

obstacles for plastic deformation, exceeds a critical threshold [44].

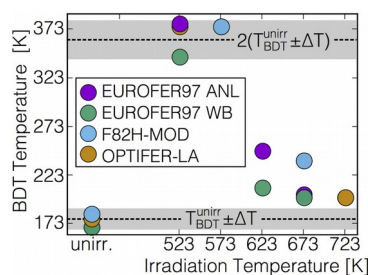


Fig 7: Temperatures of brittle to ductile transitions (BDT) in several fusion steels [45]. A model [44] based on the analysis of screw dislocation mobility suggests that the BDT temperature doubles if irradiation is performed at relatively low temperature.

For the qualification of material damage and experimental validation of models, a significant amount of experimental analysis was performed, e.g. the development of techniques for nanometer-scale experimental characterization (W, FeCr), scanning transmission electron microscopy, positron annihilation spectroscopy for defects in W, small angle neutron scattering (SANS) for defect size distribution in irradiated EUROFER97, correlation of defect structure and magnetic changes (Fe, FeCr), in-situ electron microscopy of dislocation mechanisms in W-alloys and the development and maintenance of the ion irradiation facility DiFU in Croatia.

Next to the question of generation of damage in simple microstructures, being still a pioneering development, the investigation of damage production in dislocation microstructures is in progress with the aim to arrive at a formulation suitable for applying to materials with complex microstructures, e.g. steels. The emphasis on microstructure, modelled and analyzed as a three-dimensional entity, including its dynamics derived from radiation effects, is firmly on its way to become between materials science and engineering design data.

4. Outlook

The main objectives for next European Framework Program (FP9) include the increase of engineering data base for the three baseline materials, i.e. closing gaps in the material property handbook and decreasing uncertainties in, performance limits after neutron irradiation. This requires significantly increased resources for implementing various irradiation campaigns in MTRs up to neutron fluence representative for DEMO. Accompanying programs with multi-ion beam irradiation and irradiation modelling are mandatory to increase knowledge in property changes typical for fusion environment and to reduce uncertainties inherent due to different neutron spectra.

Post irradiation examination results on advanced steels and high heat flux materials from campaigns underway will allow to select few options for risk mitigation to be investigated in parallel to baseline materials. Thereby, increased efforts towards technology are needed, i.e. the

candidate materials, both baseline and risk-mitigation options have to be industrially manufactured in larger batches and characterized as well as bulk or joint material and in combination with functional materials like barriers and coatings.

The development of DEMO specific Design Criteria and design methodologies for in-vessel components are essential for best selection of engineering options and mandatory input for safety analyses (precursor to any nuclear licensing). This as well needs strong support from verification experiments and simulations applying multi-physics and irradiation modelling.

All this work has to be done on an international perspective with a focus in particular on the future continuation of the cooperation of Europe with Japan actually performed within the Broader Approach.

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