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Fusion has entered the engineering era. Moving from plasma science to experiments demonstrating the benefits of modified torus shapes and advanced divertor geometries, the 'field' has become an 'industry'. Investors focus now on whether superconducting magnet joints are feasible in large tokamak designs and how to deliver net energy to grid. As with all technology trajectories, materials are the key enabler. For fusion materials, the three big challenges remain resilience to the combined damage effects of tritium, transmutation and neutron bombardment (a veritable 'triple whammy'), achieving suitable irradiation strategies for adequate damage studies (with optimal use of modelling as complementary science) and defining material safety and waste guidance in an era of evolving regulation.

Tritium, transmutation and neutron bombardment ('the triple whammy')

Materials in fusion reactors face a demanding combination of megaNewton (MN) linear and torsional forces, electromagnetic fields heading towards 20 tesla, high (>500°C) and low (cryogenic) temperatures and the corrosive environment of supercritical gas or molten salt / metal coolants, all coupled with a requirement for components to function in a highly precise manner for extended periods of time. However it is not performance under these stresses which dictate the choice of materials for tokamaks, but primarily the microstructural factors which determine structural (e.g. mechanical) and functional (e.g. superconductivity) resilience in the face of i) multiple atom displacements by neutrons, ii) distortions due to ingress, retention, and release, of hydrogen isotopes (especially tritium) and iii) the evolving composition of the materials (with resulting helium gas and transmutation products) through neutron-induced transmutation. Fission studies, in recent decades, define a typical damage range in displacements per atom of up to 0.1 dpa. By contrast, the UK's anticipated Spherical Tokamak for Energy Production (the STEP prototype powerplant, due 2040) will run with neutron energies and fluxes likely to inflict damage of the order of 20 – 200 dpa at first wall. DEMO (the European Community's 2050 fusion DEMOnstration powerplant project) currently sets thresholds for baseline material selection at 15 dpa per full power year, for front wall steel damage in the breeder blankets [1]. In recent years, the commercial sector has made significant contributions to fusion developments not least because the projects are small and flexible: Tokamak Energy (with their pulsed copper ST40 spherical tokamak in the UK and a future HTS fusion demonstrator concept) and Commonwealth Fusion Systems (working on SPARC in North America) are both now focussed on improved High Temperature Superconductor (HTS) magnet materials for application in fusion. While the International Thermonuclear Experimental Reactor (ITER) is an important global programme it has faced challenges with its massive scale, enormous cost and multinational partnerships, leading to limitations in innovation and evolution.

It is the structural materials, first and foremost, that will enable higher thermal operation of the fusion powerplant but since fission's next generation of advanced modular reactors also require steels operating above ~500°C, there are synergies for research in the broader nuclear community. Fission and fusion studies on irradiated metals now run in parallel, although commercial realisation of reactors is likely to be sequential: Light Water Reactors (LWRs), Small Modular Reactors (SMRs), Advanced Modular Reactors (AMRs), and then fusion.

With irradiation, metals develop dislocation and cluster-type defects. A major avenue of development is that of defect sinks via oxide dispersions - nanoscale precipitates to focus and 'defuse' the growing dislocations under neutron impact or grain boundaries. Oxide dispersion strengthened (ODS) steels are joined by complex nanostructured alloys, high entropy alloys (HEAs), and maraging and thermomechanical steels in a growing field of manipulated microstructures, to exploit differential strain, for example, to limit catastrophic damage at up to 14 MeV neutron energies or to enhance kinetics and defect behaviour to encourage defect recombination (e.g. in HEAs). To limit transmutation damage (as one element or isotope evolves to another via ongoing neutron capture), fusion materials designers also aim to constrain compositions to those elements which do not transmute under neutron impact. Resulting products include the reduced activation ferritic-martensitic steels (RAFM structural materials) which require further work related to joining techniques and improving the consistency of manufacturing quality at an industrial scale.

Early work looking to address the impact of surface damage by neutrons, on tungsten's subsequent ability to retain and release deuterium (a precursor to tritium as fuel) – suggests some degree of saturation of defects may be likely [2, 2a]. Thermal cycling in the fusion reactors of the future may also provide some annealing relief to damaged components and treatments to limit the formation of dust that may pose a radiological hazard. However, beyond saturation and stress relief, materials science must also look to sacrificial phases and suitable evolution of phases *in situ* to provide novel routes to extend component lifetime opportunities to design engineers.

Functional materials are also being targeted for development in addition to the aforementioned structural materials. The limited space within a number of designs of fusion reactor has pushed engineers to consider highly efficient shielding materials to protect high temperature superconducting magnets that control the fusion plasma, as well as components targeting and enabling the optimised breeding ratio of fuel in the fusion reactor to sustain the fusion reaction. This includes the use of Li-containing components such as Li_2TiO_3 [2b] and neutron multiplying materials containing isotopes of Be and Pb [2c]. Efficient absorber materials based upon borides (ideal for the efficient absorption of thermal neutrons), for example tungsten borides [2d], are being considered alongside other high neutron cross section materials and gamma shielding materials with high Z values.

To deliver solutions, the experimentalists require laboratories and suitable samples to accelerate innovation and the development of mechanistic models that will efficiently predict safety margins and long-term behaviour. In fusion, this implies irradiation strategies.

Irradiation strategies: testing facilities and modelling proxies

Neutron source facilities offering low fluxes at high neutron energies enable much-needed nuclear data experiments and neutron cross-section datasets that underpin shielding specifications, component lifetime estimates, waste calculations and diagnostics viability. Only a handful of these exist worldwide (including the High Intensity D-T Fusion Neutron Generator [HINEG]) in China, and Germany's DT Neutron Generator at the Technical University of Dresden (NG TUD). These will be augmented in the UK when the University of Birmingham commissions a High Flux Accelerator-Driven Neutron Facility in 2022. Novel rigs utilising benchtop and commercially available small neutron sources are also very much of interest to the R&D community, with Japan leading the way on the latter [3]. The commercial sector is also bringing low and intermediate neutron sources to the market, for example the Alectryon 300T device from Phoenix LLC.

However, research to fully understand true surface and bulk damage in fusion materials is hampered by the absence, globally, of neutron sources providing both high energy (14 MeV) and high flux (greater than 10^{14} n/cm²/s). In a tokamak, the neutron spectra across the profile from first wall to vacuum vessel change according to the type of materials present, the coolant, and component design. Such changes, especially in the percentage of thermal and fast neutrons, will have significant impact on, in general, Primary Knock-on Atoms (PKA) that cause the initial radiation damage as well as impact transmutation rates (especially when coupled with moderating materials). While the fission community provides a suite of international materials test reactors with high neutron energies, fluxes are low by fusion standards and PKA replication poor, and irradiation campaigns therefore require long exposures: each sequential year buys another dpa or two. The fusion community has a planned facility in the form of the International Fusion Materials Irradiation Facility - DEMO Oriented NEutron Source (IFMIF-DONES) which started in 1994 but realisation is not expected until 2029 and there are similar lags in the pace of financial investment. Dual-beam proton source experiments sometimes act as proxies and may offer the benefit of combined load (irradiation and mechanical load) evaluations. Ion proxy irradiations offer better temperature control on damage experiments, for modellers seeking to utilise resulting data for mechanistic simulations (including atomic scale simulations).

For the past decade or more, modelling *has* become a mainstream proxy to irradiation itself, with atomistic levels of understanding of the mechanisms of damage now mainly based on density functional theory and classical molecular dynamics simulations. This solid state physics approach has highlighted the benefits of body centred cubic (bcc) vs face centred cubic (fcc) crystallography in reducing dislocation slip in some materials and demonstrated dimensional changes can result purely from stress relaxation effects in lattices exposed to neutron impact *in silica*. Models to understand the anomalous decomposition of tungsten alloys and steels under irradiation are needed to predict the combined effects of dose, temperature and stress, for ITER, STEP and DEMO. Predictive atomic-scale algorithms for computing microscopic stresses, strain and swelling of tungsten, steels, beryllium and other down-selected baseline materials are being funded by the same international community that is building ITER. However, it is the multiscale models that take priority as urgency grows to support design engineering finite element models and failure analyses. Component-level simulations are planned, relating dose, temperature and stress - derived from the analysis of microscopic and mesoscopic models for irradiated microstructures and validated using ion irradiation experiments (aided by digital image correlation) and other integral testing.

Beyond damage and failure mode analysis, modelling must also look to augment process innovation, *in situ* monitoring and probabilistic design in the absence of traditional (fission type) design codes. This brings other materials' needs for sensor development as well as analysis of big data, machine learning and other aspects of convergence science that need to be brought to bear on solving the engineering needs of fusion power.

Defining material safety and waste guidance in an era of evolving regulation

ITER engineering design codes currently look to the fission approach and require significant data for qualification of materials, premised in the first instance, on the development of suitable small-scale test techniques. The burden of proof includes multiple industrial heats, ASTM or other certified testing standards for all data, testing results for the full operation range (in minimum 25-50 Kelvin steps), non-destructive testing verified for joint performance, development of function specific codes, cycling effect data and demonstration of negligible creep under irradiation.

Fission-to-fusion extrapolations have limitations though: DEMO has already noted underestimates in embrittlement when the fission community used Reaction Pressure Vessel data to predict Light Water Reactor degradation via formulaic extrapolation. The latter prompted risk mitigation surveillance programmes in LWR's and has led DEMO to prohibit formulaic degradation principles for licensing going forward [1].

In the UK, opinion is evolving: To bring fusion powerplant prototypes online by mid-century, traditional nuclear codes for materials acceptance and qualification will need to be replaced by a more creative – but robust – approach, potentially including *in-situ* surveillance in the first prototype reactor which will be needed *in operandi* in the reactors eventually used commercially, relying on advances in sensor and control systems (including with artificial intelligence) over the past decade or so. Alternatives to the R5 /R6 codes so well maintained by industry mainstay EDF may include pre-qualification proof testing on components in geometries designed around in-operation maximum stress areas, an approach advocated, for example, by Waldon *et al.* [4]. In the USA, fusion design code development was recently triggered within the ASME Section III organisational structure, via creation of a new sub-group for “Fusion Energy Devices”. The latter is tasked to consider both magnetic and inertial confinement and an early roadmap has been constructed to provide direction and concepts for the new Section III, Division 4 Code Rules.

From a waste regulation perspective, materials selection and design criteria will need to move beyond safety to also take account of the increasing emphasis, this century, on sustainability. With reference to the latter, a research focus will be how to reduce materials' tendency to dust formation during recycling processes, as dusts present a particularly high safety risk during these operations on first wall components. Studies in isotope partitioning methods (gas centrifuging; metal vaporisation and ionisation followed by electromagnetic separation) are experiencing a resurgence as routes to lower level waste classifications for potential fusion materials: isotopes with lower half-lives are targeted both in materials development upfront, but also in recycling of waste post-operation. As fusion looks to develop a dedicated and fit-for-purpose regulatory framework, it must look to accommodate the coming decade's material science innovations that reduce disposal and storage burdens, and tackle the application-specific topic of detritiation. Japan's risk-based approach is viewed as a positive example of what is possible.

The benefits of developing a fusion materials strategy, including the UKAEA led Fusion Materials Roadmap, will not only accelerate the development of fusion energy technologies to combat the climate emergency, but will also accelerate other key technologies including those related to the space industry, both near-earth satellite technologies and beyond-earth exploration and missions, as well as enhance other sustainable, clean energy systems including fission-based Advanced Modular Reactors (AMRs), some of which need similar leaps in material development and radiation testing facilities. Fusion facilities will enhance international collaboration at a time when it is clear that global problems such as climate change can only be solved when experts come together to support a common goal.

References

[1] Stork, D., Agostini, P., Boutard, J-L., Buckthorpe, D., Diegele, E., Dudarev, S.L., English, C., Federici, G., Gilbert, M.R., Gonzalez, S., Ibarra, A., Linsmeier, C., Li Puma, A., Marbech, G., Packer, L.W., Raj, B., Rieth, M., Quang Tran, M., Ward,

- D.J. and Zinkle, S.J. (2014), *Materials R&D for a timely DEMO: Key findings and recommendations of the EU Roadmap Materials Assessment Group*, Fusion Engineering and Design 89, 586-1594.
- [2] Hollingsworth, A., Barthe, M.-F, Lavrentiev, M.Yu, Derlet, P.M., Dudarev, S.L., Mason, D.R., Desgardin, P., Hess, J., Davies, S., Thomas, B., Salter, H., Shelton, E.F.J., Heinola, K., Mizohata, K., De Backer, A., Baron-Wiechec, A., Jecu, I., Zayachuk, Y., Widdowson, A., Meslin, E. and Morellec, A. (2021 submitted), *Comparative study of deuterium retention and vacancy content of self-ion irradiated tungsten*, Journal of Nuclear Materials "ICFRM" special edition.
- [2a] S.C.Middleburgh, R.E.Voskoboinikov, M.C.Guenette and D.P.Riley (2014), *Hydrogen induced vacancy formation in tungsten*, Journal of Nuclear Materials Volume 448, Issues 1–3, Pages 270-275.[2b] S T. Murphy (2014), *Tritium Solubility in Li_2TiO_3 from First-Principles Simulations*, J. Phys. Chem. C 2014, 118, 51, 29525–29532.
- [2c] M.L. Jackson *et al.* (2017), *Defect processes in Be_{12}X ($\text{X} = \text{Ti}, \text{Mo}, \text{V}, \text{W}$)*, Nucl. Fusion 57 086049.
- [2d] M Athanasakis, E Ivanov, E del Rio, SA Humphry-Baker (2020), *A high temperature $\text{W}_2\text{B}-\text{W}$ composite for fusion reactor shielding*, Journal of Nuclear Materials Volume 532, 152062.
- [3] Bakr, M., Masuda, K and Yoshida, M. (2019), *Improvement of the Neutron Production Rate of IEC Fusion Device by the Fusion Reaction on the Inner Surface of the IEC Chamber*, Fusion Science and Technology, 75:6, 479-486.
- [4] Waldon, C., Morrell, R., Buckthorpe, D., Davies, M. and Sherlock, P. (2009), *Engineering Practices for Tokamak Window Assemblies*, Paper 75858, 17th International Conference on Nuclear Engineering, July 12-16th, Brussels, Belgium.

