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Modelling of advanced structural materials for GEN IV reactors

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Abstract

The choice of suitable materials and the assessment of long-term materials damage are key issues that need to be addressed for the safe and reliable performance of nuclear power plants. Operating conditions such as high temperatures, irradiation and a corrosive environment degrade materials properties, posing the risk of very expensive or even catastrophic plant damage. Materials scientists are faced with the scientific challenge to determine the long-term damage evolution of materials under service exposure in advanced plants. A higher confidence in life-time assessments of these materials requires an understanding of the related physical phenomena on a range of scales from the microscopic level of single defect damage effects all the way up to macroscopic effects. To overcome lengthy and expensive trial-and-error experiments, the multiscale modelling of materials behaviour is a promising tool, bringing new insights into the fundamental understanding of basic mechanisms. This paper presents the multiscale modelling methodology which is taking root internationally to address the issues of advanced structural materials for Gen IV reactors.

1. Introduction

Determination of the life-time of components exposed to severe environments such as fission or fusion plants is very demanding, particularly when damage interactions must be considered. Over the years various attempts have been made to obtain physically based life-time assessments, however, these design methodologies still follow simple concepts such as the linear life fraction rule [1]. For the development of new materials, a better knowledge of their expected service behaviour would be extremely advantageous. Acquiring long-term statistically secured design data for complex loading conditions including damage interactions from experiments is currently impossible. It is particularly difficult to judge the long-term properties during the phase of materials development or optimization.

Issues that need to be investigated and understood for such components include creep, swelling, fracture, fatigue, cracking, corrosion, impurity effects and the correlation between nano- and micro-structural features. It becomes clear that a higher confidence in life-time assessments of these materials requires an understanding of physical phenomena on a range of scales from the microscopic level of single defect damage effects all the way up to macroscopic effects. To overcome the limitations experienced in current

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experimental setups, the multiscale modelling of materials behaviour is a promising tool, which not only addresses long-term behaviour, but also provides a fundamental understanding of materials. It has a predictive aspect of materials behaviour, probes beyond currently possible experimental approaches and allows the set-up of better tuned experiments. In the distant future, it is envisaged that development of tailor-made alloys and ceramics with optimized composition would be possible with input from accurate materials modelling.

Visible damage is usually understood as a macroscopic event like cracking, heavy plastic deformation or visible corrosion attack. For a designer the link between the atomistic and microscopic dimensions is often overlooked, although the microscopic phenomena are in part responsible for the macroscopic failure. This is compounded by the fact that design needs design curves which until now have been based on a set of experimental data which modelling currently cannot deliver. The aim of this paper is to bridge the ideologies between microscopically and macroscopically important phenomena to obtain a more robust scheme in which to predict material life-times.

To realise such a scheme, it is necessary, at an international level, to include modelling as a constitutive part of materials research. The simulation of materials under extreme conditions needs to encompass broad time and length scales starting from atomistic descriptions of primary damage formation and ending with a description of bulk property behaviour at the continuum limit. A single code running on the supercomputers of today or even those available in the future cannot describe all these phenomena. Instead, one needs a multiscale, multi-code modelling approach that begins at the atomistic level with ab initio, Molecular Dynamics and Kinetic Monte Carlo techniques, moves through the meso-scale using dislocation dynamics, and ends with the macro-scale using finite element methods and continuum models. Such large multiscale modelling strategies are finding seed internationally in fusion and fission groups. This paper will outline and discuss the possibilities and scales of materials modelling in terms of these modelling schemes with respect to advanced Gen IV reactors [2].

2. Problems of current design procedures

Components of plants and equipment operating under extreme conditions are usually subjected to a variety of exposures leading to damage and ageing of the materials used. Safe operation of components requires methods which predict materials degradation as accurately as possible. In applications where the components are easily accessible and typical maintenance intervals are short (e.g. automotive applications) or where nondestructive evaluations are easily performed during service, investigation of components taken out of service prematurely or experience by failure help to improve the reliability of a certain design. This approach for design optimization, however, fails for long-term applications (50 years and more) and for components which cannot be exchanged (e.g. reactor pressure vessel).

Design in general is based on a set of experimental data created in a laboratory and a set of design rules, codes and standards which take specific loading conditions and safety margins into consideration. Complex service exposure conditions like combinations of high temperature, irradiation, hostile environment, unidirectional and alternating stress lead to long-term damage interactions which cannot be accurately mapped under laboratory conditions or even with component testing. States of stress, actual environment, local microstructure, stress–strain–temperature history and exposure time are most important amongst them. Fig. 1 schematically illustrates the usual design procedure. Once the geometry of a component has been defined the stresses and strains are determined by finite element calculations. These calculations are based on material properties (determined in the laboratory) and material laws (constitutive equations). Design rules and code cases are used to include complex loading

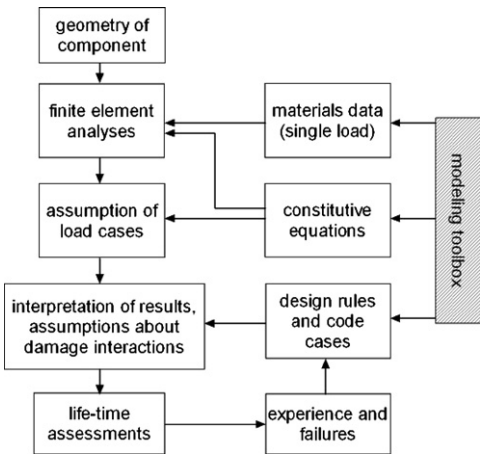

Fig. 1. Material modelling toolbox to support the design process for components operating under complex loading conditions.

situations, uncertainties about materials behaviour and damage interactions.

Even once such a scheme has been built up, it is questionable as materials' properties can change as a result of service exposure which usually leads to a degradation of properties. The causes of degradation are diverse and to give the readers an idea of what types of degradation are possible, Table 1 lists the most relevant damage phenomena which can occur in components operating under high temperatures in irradiation environments (taking an advanced very high temperature reactor (VHTR) environment as an example).

Considering these complex and long-term dependencies it becomes clear that the necessary set of accurate experimental data cannot be provided within a reasonable time at affordable costs. The only possibility until now has been to include rather simple damage and damage interaction rules together with high safety margins. Such a scheme works to some extent for known materials where a well established set of baseline data and service experience already exists. When, however, changes to service exposures, modified materials or new materials need to be investigated, the reliability of the method breaks down. In the search to overcome such limitations in methodologies, materials modelling is a new methodology which has developed and is hoped will become a powerful tool which reaches beyond the limitations of current schemes.

Modelling can provide physically based inputs into constitutive equations and finally it can provide a very valuable input into design rules and code cases for damage interactions as is indicated on the right hand side of Fig. 1. This could be an attractive approach to increase the accuracy of life-time assessments and consequently the safety of plants. When the term modelling is used in this context, we are not describing the black box FE methodology used to date, but an interactive model, where scientists must pinpoint the relevant issues and time and length scales where this phenomenon occurs at and then implement the appropriate codes. Although failure of a component is usually considered as a macroscopic event, the main portion of damage during exposure time occurs on a microscopic and even nanoscopic level. The determination of the dependence of local mechanical properties from the microstructure is therefore of utmost importance. This indicates that a multiscale modelling approach is necessary. Such multiscale modelling schemes need to encompass broad time and length scales starting from atomistic descriptions of primary damage formation and ending with a description of bulk property behaviour at the continuum limit. This necessitates a multiscale modelling approach that begins at the atomistic level and traverses time and length scales until it reaches more general continuum models. On a first read,

Table 1
Possible sources for materials degradation during service of an advanced VHTR

Type of exposure	Expected type of damage
Temperature	Phase reactions (precipitations, particle dissolution, segregation)
Irradiation	Displacement damage (point defect clusters like black dots, loops and voids leading to swelling, hardening and embrittlement) Helium damage (bubble formation at particle–matrix interfaces or at grain boundaries) Radiation induced segregation and ion beam mixing (local alloying)
Environment (He + CO/ CO_2, H_2, H_2O, O_2 impurities)	Oxide layer (eventual softening of matrix, weakening of grain boundaries) Carburization (hardening and embrittlement due to carbide formation) Hydrogen embrittlement Degradation of fibre–matrix interface
Mechanical load	Creep damage (irradiations and/or diffusion controlled dislocation movement, void formation along different types of boundaries) leading to plastic deformation, fibre pull-out and rupture

Table 2
Physical phenomena determining behaviour of materials and related atomistic scale methodologies

Methodology	Physical phenomena
Condensation and diffusion	Phase diagram, time–temperature-phase diagram, microstructural stability
Dislocation–obstacle interactions	Effects of precipitates, dispersoids and point defect clusters on yield strength, stress rupture stress, and creep strength
Dislocation–dislocation interactions	Dislocation arrangements, yield stress (shear stress), fatigue, creep-fatigue
Point defect–defect and boundary interactions	Effects of irradiation on existing voids at boundaries (void growth, void shrinkage)
(Grain) boundary diffusion	Creep damage, segregation, toughness/embrittlement
Decohesion of lattice	Crack formation and rupture
Surface phase formation	Oxidation and corrosion

designers may feel slightly overwhelmed by such a broad scheme, however this paper will show how the different scales are related and why it is necessary to address them.

It is therefore necessary to study the types of damage described in Fig. 1, determine the physical phenomena behind such damage and decide which methodology best describes this phenomenon in order decide which code is best suited. The most important physical phenomena determining the life relevant behaviour of materials are thus listed in table format in Table 2. To discuss the principles of multiscale modelling, the paper is focused on the discussion of creep and irradiation damage although the principles on which the method is based is generic for all other phenomena.

3. A model stress–strain loop

To illustrate the possible effect of exposure due to a combination of irradiation and temperature with static or transient loads we refer the reader to Figs. 2(a) and Fig. 2(b). Fig. 2(a) shows experimental creep results for the ferritic oxide dispersion strengthened (ODS)-alloy PM2000. This class of creep resistant materials is considered as a potential candidate for several advanced nuclear applications. The data was obtained under thermal load (black points) and under in situ irradiation creep conditions (red points), for more details see Chen et al. [3]. Creep rates are plotted as a function of temperature. Two distinct regions can be seen: The (almost temperature independent) irradiation induced creep regime up to about 650 °C and the thermal creep regime at higher temperatures which follows the expected thermally activated behaviour. This experimental result allows the construction of a load cycle (Fig. 2(b)) which not only illustrates the complexity of damage interaction but which can also be used to demonstrate the power of multiscale modelling[1].

Let us assume that a section of a component undergoes displacement controlled straining during transients (which occur for example as a result of thermal induced strains during start-up/shut down). Additionally, let us assume that this section is designed to move along the elastic line (shown by the black lines in Fig. 2(b)) in a way that neither plastic deformation nor thermal creep can occur.

[1] For interpretation of color in Fig. 2a, the reader is referred to the web version of this article.

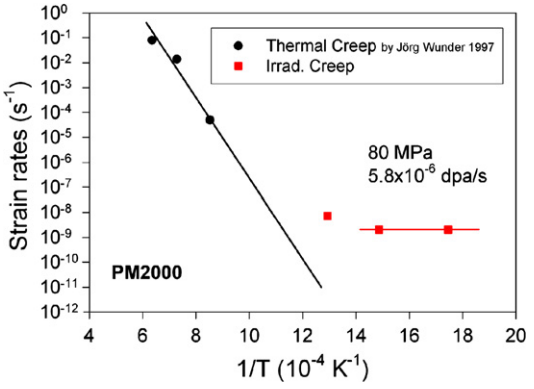

Fig. 2(a). Thermal and irradiation induced creep rates for the ferritic ODS steel PM2000 as a function of the inverse temperature (according to [3]).

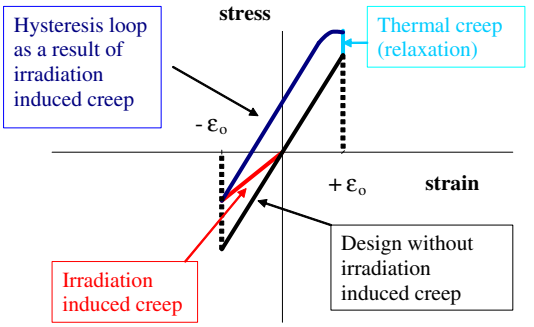

Fig. 2(b). Idealized hysteresis loop combining service relevant loads for advanced high temperature reactors to demonstrate creep-irradiation interactions.

During a temperature rise combined with irradiation, irradiation induced compression creep can occur leading to a stress well above the design stress during steady state operation which may cause thermal creep.

As many of the related effects occur on a time scale which cannot be accomplished in the laboratory, modelling such phenomena is expected to enhance basic understanding, thereby improving the accuracy of design life assessments. Rather than a logical progression of the modelling schemes starting from the smallest time and length scale and moving through scales up to macroscopic, measurable time and length scales in a bottom–up approach, we address creep as the designer understands it and studies it – top–down – looking at first at constitutive equations, then going down a scale to the interaction of dislocations and their role in the mechanical behaviour of materials and then move to smaller scales, often not visible by the experiments

undertaken and overlooked by designers, but which indeed are important to include and have indeed become a reputable methodology to provide insight into materials' behaviour.

4. Dislocation dynamics (DD)

An important question is the reliability of input data into existing FE calculations. Constitutive laws like the stress–strain curve or the creep law which are very important inputs into finite element calculations are sensitive to exposure and may change. It is envisaged that such changes will be trackable with dislocation dynamics and therefore it is of great interest to model such phenomena with dislocation dynamics simulations. Dislocation dynamics (DD) is a mesoscopic modelling method which studies longer time and space dimensions by defining a segment of a dislocation as the smallest element in the calculation. At such a scale important phenomena such as studying the cutting of forest dislocations due to their role in the shear stress of a metal can be performed. One of the aims of such simulations is to produce a DD derived stress–strain curve which has recently been achieved for molybdenum [4].

In the case of fatigue, dislocation–dislocation interactions play a central role. Experimental TEM results have shown that the typical dislocation arrangements after fatigue are dislocation bundles with single dislocations perpendicular to the direction of the bundles as shown in Fig. 3(b) for Al after fatigue load at room temperature. Fig. 3(a) shows the result of fcc DD simulations with similar results indicating that DD does indeed reproduce the results seen in experiment [5].

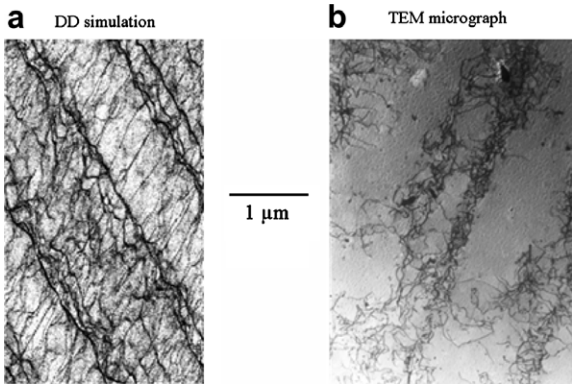

Fig. 3. Dislocation arrangement in aluminium after fatigue load at room temperature. Comparison between experiment and DD modeling. (DD results curtesy of Groma and Bakó [5]).

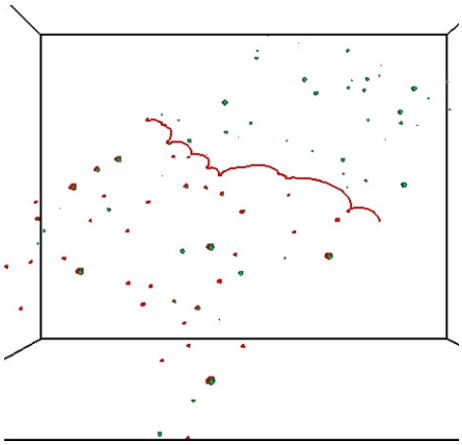

Fig. 4. Dislocation dynamics simulation of a dislocation gliding through the ferritic ODS steel PM2000. Orowan loops are left behind around dispersoids (according to [6]).

The goal to strengthen materials has lead to the development of oxide dispersion strengthened (ODS) materials. ODS metals consist of a metallic matrix (austenitic, ferritic or martensitic) containing finely dispersed oxide particles. These obstacles have been found to be the limiting factor in dislocation movement, indicating that dislocation–dispersoid interactions are the relevant phenomena to investigate in such materials. The investigation needs to have a quantitative understanding of the particle size, particle distribution, the interface between particles, eventual nano-clusters, matrix coherency and lattice mismatch. A dislocation dynamics simulation of the commercially available ferritic ODS alloy PM2000 (Plansee) is shown in Fig. 4 [6]. The sample was constructed from information on particle size and distribution obtained from experimental TEM analysis [7]. The green spheres represent the dispersoids present in the material and the red lines indicate the dislocation. The figure clearly shows that the dispersoids pin the dislocation and indeed in some cases leave an Orowan loop encircling the dispersoid. Such a deformation mechanism is in agreement with experimental findings [8] at low temperatures. To develop these simulations further so that one can model components in advanced reactors, such as the VHTR, it will be necessary to introduce mechanisms acting at higher temperatures like dislocation climb and even diffusion controlled creep mechanisms which are currently not in the DD code[2].

[2] For interpretation of color in Fig. 4, the reader is referred to the web version of this article.

5. Molecular dynamics (MD) and kinetic Monte Carlo (kMC)

DD simulations do not include the microscopic interaction known between dislocations and defects. Such details need to be studied using Molecular dynamics (MD) simulations. Molecular dynamics implements the Schrödinger equation to describe the movement of atoms in space and time as a results of interatomic and external forces. MD studies of dislocation–defect interactions with nano-sized particles [9] and voids [10] have shown that the dislocation–void interaction depends on dislocation velocity, dislocation density, applied stress and temperature. Such results are important as input parameters for DD simulations. The use of MD alone, however, as an alternative to DD, is not possible as it probes very high strain rate interactions and cannot model climb or diffusion mediated bypass, such that individual use is insightful but complementary use of codes at different scales enhances results and understanding tremendously.

Other phenomena which are of great interest at an atomistic scale are the kinetics of vacancies, interstitials, clustering and cascade ageing and diffusion which can be studied using a combination of MD and kinetic Monte Carlo. Kinetic Monte Carlo method (KMC) is a probabilistic approach that enables one to predict longer term damage evolution. The output data of MD, is used in KMC in order to determine the probabilistic motion and reaction between defects [11,12], where motion and clustering of point defects are the dominant mechanism. Such results on damage evolution give a picture of the effects of irradiation which also contribute to creep at low temperatures. For example, let us assume that as a result of thermal creep grain boundary voids develop. Production, growth and their coalescence govern creep rupture behaviour. Returning to Fig. 2(b), let us assume that displacement damage takes place during the start up of a reactor, resulting in the interaction with creep voids present from the preceeding thermal creep phase. One aspect of interest is to study how these voids grow. MD simulations producing irradiation of nanocrystalline iron which contains a pre-existing void in the grain boundary has shown that interstitials move to sinks present in the material – i.e., to both the grain boundary void and to the grain boundaries themselves [13] (Fig. 5). No comparative difference could be seem between the sink strength of a void or neighbouring GBs. Unfortunately the time limitations of the MD simulations does not provide the possibility to study the movement of vacancies, such that the future of the void, where it will act as a stronger sink for vacancies and grow, which one would expect from experimental results, can not be resolved on the MD timescale and necessitates a KMC study. To bring these simulations back into the design perspective in regards to the issue of creep or fatigue damage, such simulations provide information on the point defects which affect the deformation behaviour which in turn has an influence on grain boundary sliding (creep) and slip (fatigue) and is therefore a necessary study to undertake in order to understand mechanical behaviour.

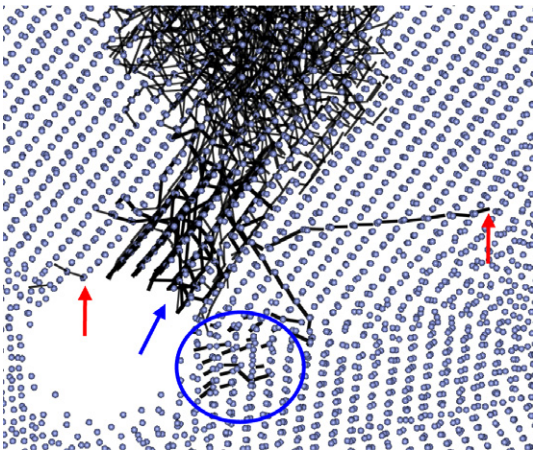

Fig. 5. Section of MD simulation showing a pre-existing grain boundary void. Black lines indicate the movement of atoms during irradiation. Red arrows indicate where atoms move away from the void. Blue indicates where atoms move towards the void (see also [13]) (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.).

6. First principle considerations

We have emphasized that in order to produce quantitative rather than qualitative results from the simulations it is necessary to start at the fundamentals and build up the input from one level to the next. In order to obtain realistic results from MD simulations we need to question the reliability of the potentials they need as input. This is possible by performing first principle ab initio calculations to obtain data on the interatomic forces which are present between atoms. Such calculations are limited to a small number of (up to a few hundred) atoms. These results, which at a first glance seem

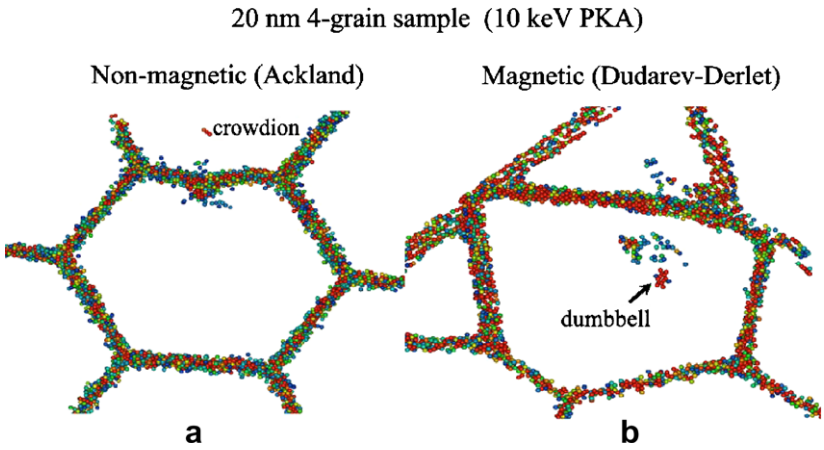

Fig. 6. Section of the MD sample (only showing GB atoms using an energy cutoff criterion) after relaxation of the same displacement cascade (10 keV PKA), introduced in the sample at the same atom, with the same angle using the (a) non-magnetic Ackland potential and (b) magnetic Dudarev–Derlet potential (see also [15]).

far removed from design, actually are extremely relevant as they are used, along with any experimental data available to produce the interatomic potentials which are used as input data in larger scale simulations. If the ab initio results are not calculated adequately, then any further simulations will be limited by the input provided from these results, such that without a stable foundation, the entire multiscale calculation one performs will not provide a realistic picture. This means that all these larger scale simulations are only as good as the potential allows them to be. One example is the effect of magnetism in the case of ferritic steels. Magnetism has been overlooked in the past in order to simplify calculations, however, recent ab initio calculations of Fe revealed that magnetism influences the movement of defects [14] and will therefore affect the defect structure of materials. This influence can be seen by comparing displacement cascade MD simulations using non-magnetic (Ackland potential) and magnetic (Dudarev–Derlet potential) potentials which show differences in number of defects, cascade volume and result in different GB movements (Fig. 6) [15]. Once antiferromagnetic Cr is included to the Fe matrix the situation becomes even more complicated, with experimental [16] and computational [17] results revealing that magnetism is the cause of changes in the clustering as a function of the Cr concentration, which in turn affects defect configurations and mobilities. Potentials for magnetic materials, should therefore include magnetism. For Fe, the first magnetic potential [18] was published only as recently as last year, such that past non-magnetic simulations need to be re-assessed to address the role of magnetism.

Such effects indicate the necessity to properly evaluate important issues of the particular material under review with the knowledge of designers, modellers and experimentalists in a combined effort. Different phenomena then need different approaches due to the scale of the phenomenon. A designer needs to have a good knowledge of the material and then tailor the various codes at various scales in order to properly reproduce the important and relevant factors for their material of study. This emphasizes the need to understand the material on various time and length scales, pinpointing the relevant factors and focusing on these.

7. Outlook for the future of components for gas cooled reactors

Let us now summarize the most important factors which need to be addressed for VHTR and GFR components.

7.1. Reactor pressure vessel

It is assumed that the RPV will be made of an advanced martensitic 9% chromium steel (T91). As a result of temperature and eventually irradiation, microstructural changes and embrittlement can occur. To understand such materials it would be ideal to study Fe–Cr–C. Current modelling studies are performed on Fe–Cr. Magnetism in this case is a very important factor that needs to be properly

understood and implemented. Recently, studies on the complex inclusion of carbon in the Fe system have begun in a first step to study steel.

7.2. Reactor internals

New grades of materials (e.g. ODS) are considered as reactor internals, despite the well known austenitic steel 316. The ferritic Fe–Cr–C system (plus alloying elements) together with dispersoids, irradiation induced creep and thermal creep, creep-fatigue irradiation effects are the relevant processes to study.

7.3. Piping and intermediate heat exchanger

These components are outside the reactor and therefore irradiation effects do not need to be considered. Ab initio considerations have to be extended to FeNi (e.g. for 800 H) or NiCr (IN-617). Creep, fatigue and surface reactions are the life limiting factors in this case. ODS materials are also possible candidates for very advanced concepts. Mechanical performance, production and forming issues like optimization of dispersoids or subgrain formation must be studied.

In order to model each component it is necessary to define the important factors in each case. Instant results are not promised; what is expected is a gradual inclusion of results into design considerations. The necessary development time for advanced Generation IV systems could provide the necessary lead time to make such an approach a success.

8. Discussion and conclusion

Modelling materials behaviour in principle has the capability of increasing the predictive capability of materials exposed to extreme conditions, thereby minimizing the risk of premature failure of components and plants. A brief look at how creep and irradiation damage can be modelled in this multiscale story shows how component and materials design could be tackled. This multiscale scheme is far from complete and is at a far off stage from being directly incorporated into design rules. Time scales are very short, modelling temperatures are low, long-term effects and effects of high temperatures are not yet developed. Model development can only become successful together with experimental validation of first elementary structures, indicating extra work for experimentalists as they need to go back and perform tests on non-industrial materials to validate these models. For applications, which need long-term predictions of damage under complex loading conditions like future nuclear fission plants, the current status of multiscale modelling is not adequate for direct application to design procedures as it is still in development, however even at this stage it is possible to obtain much insight into mechanisms that are present in materials. Such a modelling scheme will benefit most by bringing together an international consortium of modellers, experimentalists and designers to work together in determining important factors, how to best tackle them with currently existing and/or new codes and methodologies, and to iteratively validate these models with experiments which are directly comparable to improve them. These models need to use codes which best describe the scale of the phenomenon and incorporate smaller scale input to produce quantitative results. If a robust modelling toolbox is constructed on a stable foundation, then a very interesting materials program will be possible in the future for the life-time prediction of materials.

Acknowledgements

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