Journal of Nuclear Materials 392 (2009) 286–291

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Advanced materials modelling – E.U. perspectives

M. Samaras *, M. Victoria, W. Hoffelner

HT-MAT, LNM, Nuclear Energy and Safety, Paul Scherrer Institute, 5232 Villigen, Switzerland

A B S T R A C T

Modelling of advanced materials has become a main tool in materials development. This is particularly the case for present developments in advanced nuclear materials. This paper reviews the current status of modelling fuels and structural materials in the EU and discusses future programs. At the microscale, fundamental physics issues such as magnetism are being included to build a robust modelling scheme and to understand microstructural stability. At the meso-scale, dislocation interactions with defect clusters, void/bubbles and dispersoids are shown to be the main cause of hardening. How such issues, as well as model validation experiments are emerging to verify these modelling schemes is presented.

1. Introduction

Today, it is realised that to address the global rise and continual increase in energy consumption and climate change, a safe, peaceful implementation of nuclear energy will be one of the diverse sources which will help to ease the strain on current energy resources due to the current lack of alternative technologies to address this issue. The EU is addressing such challenges by focusing efforts into large, European-wide coordinated activities with funding provided through Framework Programs (FP). These programs wish to focus the research and development performed on new technologies at a European basis by stressing international collaboration, as well as emphasizing knowledge databases, education and training. Such framework programs have been running since 1984, with 4–5 year durations. FP6 ran 2002-7 (with some programs given limited extensions). The first programs for FP7 started in early 2008 and others, if accepted, will begin in the forthcoming months and will run until 2011 with possible extensions to 2013. The nuclear component of research is enveloped in Euratom [1], within the FP programs and separates its activities into fusion, fission and radiation protection, and nuclear JRC (Joint Research Centre) sections [2]. These research activities include large experimental programs with facilities such as JET (Jet European Torus) [3], ITER (International Thermonuclear Experimental Reactor) [4], and a focus on the entire nuclear fission fuel cycle to obtain enrichment, reprocessing, waste treatment, storage, disposal and radiation protection.

The lifetime assessment of advanced nuclear materials, both structural and fuels, requires an understanding of their behaviour on a range of scales. Materials scientists are faced with the scientific challenge of determining the long-term damage evolution of materials under various extreme conditions. To understand such phenomena it is thus necessary to study phenomena such as creep, swelling, fracture, fatigue, cracking, corrosion, impurity effects and the correlation between nano- and microstructural features, as well as the effects of irradiation. To overcome lengthy and expensive trial-and-error experiments or irradiation campaigns, multiscale modelling of materials behaviour is a promising tool which addresses the broad spectrum of processes present and brings new insights into the fundamental understanding of basic mechanisms [5].

Materials modelling [6], whether structural or fuels, is finding a firm place in many experimental programs internationally as a next step in materials development. Its predictive aspect probes beyond currently possible experimental approaches and allows the design of better tuned experiments.

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. Ideally simulations would be carried out using first principle calculations. However, such calculations are restricted to systems with a few hundred atoms at 0 K. To include temperature and larger time and length scales a multiscale modelling approach is needed. In such an approach, multiscale, multicode modelling is used that begins at the atomistic level with *ab initio* and molecular dynamics techniques, moves through the meso-scale using lattice kinetic Monte Carlo and dislocation dynamics, and ends with the macroscale using finite element methods and continuum models (see Fig. 1 for the typical multiscale paradigm). Such large multiscale modelling strategies are being implemented internationally, enabling the modelling of behavioural properties of materials which is producing breakthrough science and technology. To best use these computational tools it is also necessary to assess existing data and optimise new experiments, the results of which are

* Corresponding author. Tel.: +41 56 310 4184; fax: +41 56 310 3565.
E-mail address: maria.samaras@psi.ch (M. Samaras).

0022-3115/$ - see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.jnucmat.2009.03.016

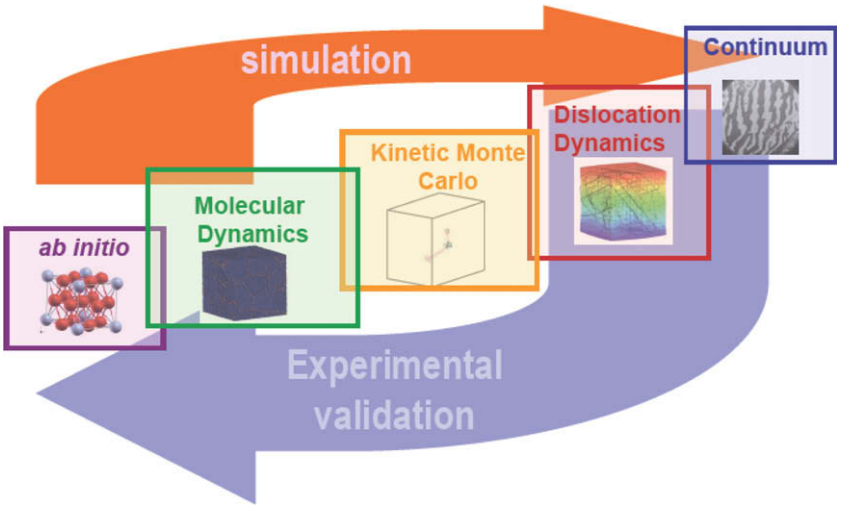

Fig. 1. Multiscale modelling paradigm showing different time and length modelling tools used in simulation and the need to validate these tools with experiments. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

incorporated into the simulation code in order to develop realistic models which will allow extrapolation beyond the existing databases for lifetime prediction. Thus, it is important to have an iterative program with complementary experiments to verify, validate and further develop the computational models.

This interchange between computational models and experiment is critical in developing accurate predictive models. By placing an emphasis on modelling, it is hoped that it will be possible to reduce the time and the experimental investment needed to develop high quality advanced materials.

Within the EU, several schemes are already underway to tackle the understanding of advanced materials through modelling and model validation methodologies. To describe the nuclear materials modelling research performed Europe-wide would be too complex a task. Therefore in this paper, the focus remains on coordinated modelling and model validation research activities performed at a European level, encompassing fusion, fission, and other EU funded projects.

2. Issues

The material's mechanical properties and changes in these properties under extreme conditions need to be understood to evaluate the candidacy of materials for use in fission or fusion reactors. In fusion reactors, structural materials will be exposed to 14 MeV neutrons, which create atom displacements accompanied by high levels of hydrogen and helium production. Within fission and including the different Generation IV reactor designs, the issues include effects of radiation damage, hardening and embrittlement (<0.6 TM, where TM is the melting temperature, and >40 displacement per atom, dpa), irradiation-induced precipitation which leads to phase instabilities (0.3–0.6 TM, 10–40 dpa), void swelling (0.3–0.6 TM, >10 dpa), high temperature He embrittlement (>0.5 TM, >40 dpa) and irradiation creep (<0.45 TM, >10 dpa). Ideally a materials' strength and toughness should undergo minimal degradation as a result of swelling and creep. As the microstructural features in materials can profoundly affect what happens on a larger scale, modelling the microstructure brings forth important results. The prominent atomic scale properties to be determined with first priority are the types of defects created, their evolution, migration and interaction, boundary structures, segregation effects, dislocation behaviour and the role of impurities. These features are needed as input for macroscopic scale continuum model simulations to study, for example, fracture, yield and creep. In fission reactors, this applies to both structural materials (pressure vessel and internals) and fuels.

The typical example of this procedure is exemplified by the effect of radiation damage exposure on the structural and mechanical properties of the material. The basis of such irradiation occurs at the nanoscale whereby an energetic atom, a Primary Knock-on Atom (PKA), induces lattice disorder in displacement cascades in the timeframe of a few tens of picoseconds. Such phenomena cannot be observed experimentally and need tools such as molecular dynamics simulations to model them. The proper interatomic potentials for such calculations are derived from Density Fluctuational Theory (DFT) calculations, as well as the basic defect properties (formation and migration energies). At the microscale, these cascades lead to a primary state of damage with the production of defects, whose evolution in turn affect the material's macroscopic properties. This microscopic evolution, the interaction, annihilation or clustering of defects, can be studied using Kinetic Monte Carlo (KMC) simulations and rate theory. The microstructure resulting from defect accumulation leads to a hardening process and in order to obtain an estimate of the yield strength which results from the interaction of these defects with dislocations, larger time and length scale models such as dislocation dynamics are used and parameters such as the critical resolved shear stress are calculated. These results are the input for continuum and finite element calculations. 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 on the microstructure is therefore of utmost importance.

What emerges is a range of structural and mechanical issues, relevant for both fuel and structural materials, all of which encompass multiscale phenomena which start at point defects and finish on long time and length scales in order to understand the lifetime of materials. These issues can be tackled with the help of modelling tools which have, are, and will be developed.

3. EU programs and groups

Of the recently finished fission FP6 programs, two included materials modelling components, Nuresim (NUclear REactors SIMulation) (fuels) and PERFECT (Prediction of irradiation damage effects on reactor components) (which dealt with Reactor Pressure

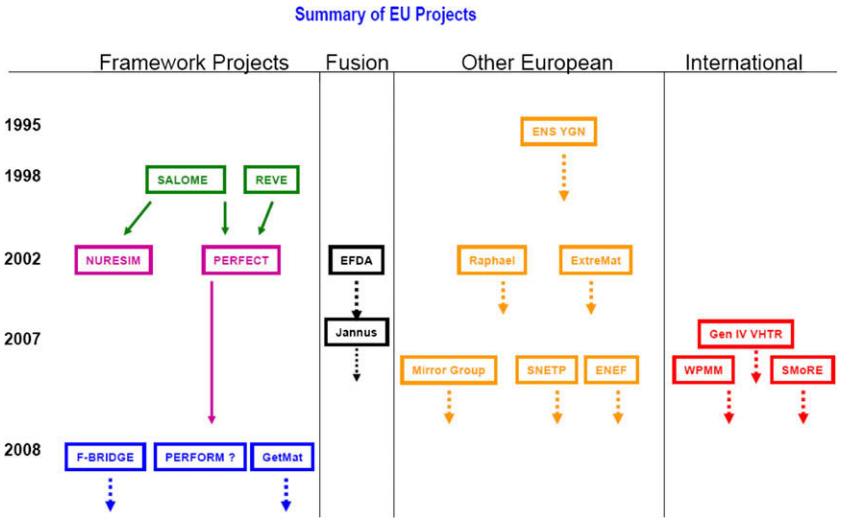

Fig. 2. Summary of EU projects from their kick-off date. Dotted lines indicate programs are ongoing. Block lines indicate that the project has flowed on to an ongoing project. Colour scheme indicates: FP5 – green; FP6 – pink; FP7 – blue; European fusion – black; other European projects which are discussed and include modelling – orange; international groups which are relevant to this diagram – red. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Vessel (RPV) steels and internals). Both of these modelling activities use a modelling basis provided in the FP5 programs of SALOME (Numerical Simulation Based on Open-source Software Architecture) and the REVE (Reactor for Virtual Experiments) project (USA, Japan, Europe). Euratom FP5 also supported the ITEM (Improvement of techniques for multiscale modelling of irradiated materials) network [7] at different EU laboratories, aimed at coordinating the development of new models and VOCALIST (Validation of constraint-based assessment methodology in structural integrity) [8] whose aim was to study the fracture of components through model development. However, since they did not develop into further projects, these two programs will not be discussed here. In the forthcoming fission FP7 programs, F-Bridge (Basic Research in support of Innovative Fuels Design for the Generation IV systems) and GetMat (GEn IV and Transmutation MATerials) (dealing with structural materials) include coordinated modelling schemes. In the fusion FP6 programs, EFDA (European Fusion Development Agreement) established a modelling program, in 2002, and continues its research into FP7. These are described from their chronological kickoff date and are summarised in a diagram in Fig. 2.

3.1. FP6

SALOME [9] is a methodology which wraps codes of varying scale inside a box with the idea that it would allow the end user to come with a problem and solve it. The numerical simulation environment was not specified, and the platform was envisaged to have a broad range of users. It enabled an easier method of exchanging data coming from different codes. However, as with all one-code methodologies, it was found to be limited.

REVE (2000–2004) [10], which aimed at simulating irradiation effects, as a virtual reactor, was also based on this one-code ideology and was interfaced in python-tk. Although it could provide an acceptable qualitative output, it needed large improvements in the physics modelling and database to make it into a predictive tool. Euratom FP5 supported the SIRENA project, aimed at applying REVE to Zr–Nb alloys.

Nuresim [11], was a continuum-based modelling scheme whose aim was to provide a Common European Standard Software Platform for nuclear reactor simulations in order to provide 'best-estimate' tools for understanding fuels of current and future nuclear reactors. The idea was the integration of multiscale multiphysics by incorporating the latest advances in reactor core physics, thermal hydraulics, and coupled (multi-) physics modelling to obtain more advanced physics and therefore improve the efficiency of the simulations. The common software platform used was SALOME. Verification and benchmarking of this code was to be performed using deterministic and statistical sensitivity and uncertainty analyses; training and quality assurance.

Among its achievements at termination, Nuresim had successfully coupled Monte Carlo codes with burn-up codes (TRIPOLI + DARWIN); was able to perform Monte Carlo investigation on decreasing the variance; and had released cross-section libraries for core calculations and advanced lattice scope tools. Issues put forth to be addressed in future work are the coupling of core physics, thermal hydraulics, and fuel models for reactor safety; sensitivity and uncertainty analysis using deterministic and statistical methods; experimental validation and qualification of codes using benchmarks, industrial plant data and results of (existing or new) experiments.

Within this program, what was missing was an understanding of atomistic processes in the materials. Without such an understanding, this large, integrated code, would still be subjected to the limits found in current design modelling – i.e., it fails to be a truly predictive tool.

PERFECT was part of FP6 (2004–2007) and produced integrated results on a multiscale modelling program dedicated to understanding the damage caused by irradiation of steels for pressure vessel and internal components. It investigated the effects of radiation damage on the material's properties which affect the material's lifetime, such as hardening, irradiation creep and void swelling, for both ferritic RPV and austenitic steel in light water reactors (LWR) internals. Within this scheme, the issues investigated were how to understand shifts in the ductile-to-brittle transition as a consequence of irradiation-induced embrittlement, to understand irradiation assisted stress corrosion cracking (IASCC), void swelling and embrittlement.

The very ambitious main concept of this European project, as in its predecessors, has been to construct a black box software system, with all the modelling results incorporated into an integrated platform which, using a set of parameters, would run the program to obtain an estimate of the issue of interest, such as fracture and corrosion, with a certain degree of accuracy and uncertainty.

To understand the mechanical behaviour of cracking, a two tier scheme using microscopic and macroscopic modelling was undertaken. The property analysis issues were separated into the topics each representing a task: physics modelling; mechanics modelling for pressure vessels; and mechanics and corrosion modelling for internal structures. These have been embodied into an integration platform which wrapped individual codes into a single code for external users.

Yet, because of the large number of variables which are necessary to solve a problem such as fracture or stress corrosion cracking on the multiscale, the complete coupling of the calculation modules was not realised by December 2007 and after a 6-month extension the integration was not totally realised. To realise these objectives a follow up has been put forth in the form of the PERFORM-60 (extension of lifetime towards 60 years) project submitted to and currently under review in FP7.

Even so, PERFECT has produced an important number of results that are described in what follows in terms of each of the tasks. In the physics modelling a number of potentials have been developed (i) an Fe–Cu potential consistent with the thermodynamics of the system [12], (ii) Fe–C potential that was used in diffusion simulations of α-Fe at low C concentrations [13], KMC methods have been used to predict the long-term evolution of defects and diffusion of impurities (Cu, Ni, Mn, and Si) in Fe, leading to the formation of different precipitates [14,15]. These results have been compared to experiments measuring precipitates and defect densities using positron annihilation spectroscopy and atom probe tomography [16,17]. The resulting types of defects were used as input obstacles into a 3D Discrete Dislocations Dynamics (DDD) code to predict the dislocation-defect interactions in bcc Fe at the grain scale and are then introduced at the grain aggregate level. A local fracture criterion is then used to predict the fracture toughness [18]. This information constitutes the result of the first module, which is then used as input to study the material mechanics. The RPV mechanics modelling module then aims at predicting fracture at a higher level as a function of loading and irradiation conditions. The main results obtained here are: (i) a micromechanical methodology proposed to derive a local probability of fracture for a representative aggregate derived from an experimentally determined carbide size distribution and associated nucleation and propagation criteria, (ii) a model of the brittle–ductile fracture toughness transition based upon continuous dislocation dynamics, (iii) local approach models were used to predict the shift in brittle–ductile transition temperature with irradiation, (iv) a theoretical basis for correlating yield stress increase and transition temperature shift, (v) development of a comprehensive materials property database, (vi) a robust method for predicting cleavage fracture toughness behaviour from Charpy-V impact test data, combining both brittle and ductile fracture local approach models.

Early in 2002, the European fusion technology programme established a modelling task within EFDA, focusing on the radiation effects in the EUROFER steel [19] under fusion relevant conditions. A concept central to the program was that instead of treating the multiscale approach as an automatic principle to apply to all length and time scales of interest, its main objective is to capture the physics of the processes occurring at each scale. Based on this premise, substantial use was made since the inception of the program of DFT, recognizing that its present accuracy provided energy values capable of clearly differentiating between different configurations.

A first application of this concept gave rise to the recognition of the importance of magnetism both in defining defect configurations in pure Fe [20] and the stability of the Fe–Cr system [21]. It was established that due to magnetism the minimum energy configuration of self-interstitials in Fe was the [1 1 0] dumbbell, while for all other bcc non-magnetic transition metals, it is the [1 1 1] crowdion [22]. Empirical potentials used up to this time did not recognise this point and lead to errors in the way in which defect formation is described in the molecular dynamic description of defects formed during the displacement cascade evolution. As a result a new Fe potential was developed [23] that, within the embedded atom formalism, described the environmental dependence of the magnetic energy and reproduced the correct ordering of interstitial formation energies.

DFT was further combined with Monte Carlo methods to calculate in Fe, not only the formation energies of defects, but also the activation energies for their migration and that of the clusters formed. It resulted in the first complete and accurate description of the low temperature annealing stages of the resistivity of electron irradiated Fe [24]. The same powerful combination, together with rate theory, was used for a very successful description of the desorption mechanisms in He implanted Fe at different temperatures [25].

At larger scales, the modelling of the role of grain boundaries as sinks for single defects and clusters produced by cascades, show that GBs are very effective for capturing self-interstitial atoms and their mobile clusters [26]. The interaction of dislocations with irradiation produced dislocation loops, voids and He bubbles, showing that small loops and voids are strong obstacles to dislocation motion, while non-pressurised bubbles are not, but their strength increases with their He content [27]. This research has received further funding and will continue for the next four years including the following issues: (i) further development of the Fe, Fe–He and Fe–Cr–He potentials and *ab initio* calculations for their use in damage accumulation studies, (ii) the modelling of mechanical properties in Fe and Fe–Cr alloys from first principles up to dislocation mechanics, (iii) modelling the Fe–Cr phase diagram using magnetic cluster expansion. The experimental validation studies include the use of the Joint Accelerators for nano-science and nuclear simulation (JANNUS) facility to study He effects in Fe–Cr, He desorption experiments to validate kinetic Monte Carlo calculations in Fe–He, and TEM studies of damage accumulation in pure Fe–Cr alloys.

3.2. FP7

The EURATOM FP7 nuclear research and training activities (2007–2011) formally includes modelling in its criteria of research activities with a strong emphasis on the advancements and long-term sustainability of materials, education, and on collaborate with the Generation IV International Forum. The programs currently accepted that contain modelling are GetMat and FBRIDGE. As stated earlier PERFORM, the follow-on project of PERFECT, is currently in review and therefore will not be discussed further.

The aim of F-Bridge (Basic Research in support of Innovative Fuels Design for the Generation IV systems), coordinated by Commissariat L'Energie Atomique (CEA), France, is to understand fuels and fuel cladding under irradiation [28]. The modelling section within this work aims at developing a multiscale methodology and characterisation tools to study UO_2 and SiC. The program aims to connect the technological issues of Generation IV systems with basic research by coupling the separate effect of experiments and modelling. There is a strong emphasis on the transfer between basic research and technological issues related to Generation IV systems and an aim to optimise the design of irradiation experiments.

GetMat (GEn IV and Transmutation MATerials), coordinated by the Forschungszentrum Karlsruhe [29], aims at understanding the synergistic effects of irradiation and environment on Fe–Cr alloys, as model alloys of ferritic/martensitic steels. This program implements a multiscale modelling approach to correlate the microstructural changes to changes in the mechanical properties. The effect of additional elements, such as C, N, Mo, Nb, V, W, Ta, and Mn is intended to be studied as well as the performance of model

experiments under well controlled experimental conditions, with the intention that both modelling and experimental validation be used for the development of technological alloys.

4. Other European nuclear energy activities

A brief description of other nuclear materials focused European activities will now be discussed.

JANNUS [30] is an experimental facility dedicated to model validation of nuclear fission and fusion materials science. With an emphasis on the teaching of irradiation effects and ion beam techniques, it was built in order to establish a facility which performs model-oriented experiments which are cost-effective, on non-active samples. In an integrated manner, it intends to provide feedback which validates multiscale models. The facility consists of dual and triple ion beams with the possibility of performing in- and ex-situ observation and characterisation. Such a facility is of high priority as a validating tool to build a robust multiscale modelling scheme. The project started in 2002, is currently in construction and first testing should be available sometime in 2008.

Extremat (new materials for extreme environments) [31] an EU FP6 Integrated project, is non-nuclear, however it contains a small component of modelling in regards to W and Fe–Cr. The EU FP6 Raphael (ReActor for Process heat, Hydrogen and ELectricity generation) [32] contains 'embryonic' modelling of graphite. Other EU platforms launched towards the end of 2007 to address modelling nuclear materials include the Sustainable Nuclear Energy Technology Platform (SNETP) [33], the European Nuclear Energy Forum (Bratislava and Prague) (ENEF) [34], and the Mirror Group whose emphasis is 'Towards a low carbon future' [35].

Europe is also involved in international/global consortia containing modelling. Within Generation IV, there is a VHTR multiscale modelling component (launched January 2007) [36]. Within the Organisation for Economic Co-operation and Development (OECD), Nuclear Energy Agency, which includes Europe, USA, Japan (launched January 2008), a 'multiscale modelling of fuels and structural materials for nuclear systems' (WPMM) [37] has been launched to study UO_2, PuO_2, MOX, SiC, Fe–Cr alloys, ODS, ferritic steel, austenitic steel, and austenitic/martensitic alloys. The International Atomic Energy Agency (IAEA) has also brought together the 'Accelerator Simulation and Theoretical Modelling of Radiation Effect' (SMoRE) project (launched December 2007) [38].

It is important to remember that the move away from nuclear has lead to a 'brain drain' of knowledge due to the lack of exchange from the generation that created the reactors used today to the developers of systems that will be created in the future, due to the retirement of many of these people. The return to nuclear has lead to the emergence of internationally-based research initiatives as well as nuclear youth organisations which aim at educating the future scientist, to build a safe and peaceful nuclear future. One such aim is to develop advanced materials which will ensure the safety of future generations through Generation IV and fusion reactors. To address this need, the European Nuclear Society Young Generation Network (ENS YGN) [39] was founded in 1995, aimed at preparing future generations of scientists with the exchange of knowledge between generations. It encompasses the 26 member countries of Europe, has been undertaking forums since 2005, and is involved in international youth conferences. The next one, the International Youth Nuclear Congress (IYNC), will be held in Switzerland in September 2009 [40].

5. Shortcomings/drawbacks

The modelling paradigm presents the methodology of the future, however in its current form it still contains limitations and drawbacks. Due to the limited number of atoms that can be studied using first principles calculations, it is difficult to study complex alloys and therefore to produce empirical potentials for complex alloys for larger scale calculations. Thus until now studies have been mostly on pure materials. The complex nature of carbon has meant that there is almost no carbon in the model alloys. This brings forth the question of when it will actually be possible to model steels. In first principles calculations, the localisation of f electrons (fuels) has led to difficulties; for example using DFT LDA (Local Density Approximation), UO_2 is predicted to be a metal. The issue of temperature in many of the calculations is still an issue. First principle techniques are currently at zero Kelvin, as are DDD calculations. MD is often restricted to intermediate temperatures, where the empirical potentials have been fitted and fail to reproduce the character of the material at high temperatures. Grain boundaries are not included in many of the meso-scale models. Charge transfer is difficult to add to interatomic potentials. For UO_2, this is a definite issue that needs to be addressed. The level of accuracy of the methodology needs to be clarified; the proper physics needs to be included. For example, when magnetism is not included in first principle calculations, then the energetics of the most stable interstitial in bcc Fe changes. Even when magnetism is included, the question then arises, should the spin-orbital moment also be included, since it plays a role. Such issues need to be investigated in order to avoid the requestioning of such issues in the future, which would lead to the necessity to perform the same work again. Diffusion is an issue which has not yet been tackled properly. Diffusion affects the microstructure of the materials, depending on the temperature and elements that diffuse for example to GBs and degrade the mechanical properties of the material. Entropy is also difficult to calculate from first principles.

The modelling scale is at such a level that the measurement techniques for validating simulations is difficult and often there is a gap between modelling and measurement. Such experiments need high purity model materials so that a proper comparison to theory can be performed, however these experiments are difficult to perform and require a strong coordination between experimentalists and modellers. To what extent can these experimental materials be 'dirty' and still produce results which can be compared with the modelling in question? Such issues need to be addressed and considered when tuning a modelling and experimental validation program.

6. Conclusion

In the distant future, it is envisaged that development of tailor-made alloys and ceramics with optimised composition for nuclear application will be possible as an outcome of synergistic materials modelling and model-led experiments. To address such a challenge, the EU has already started integrated programs through European-based International Framework Programs.

These multiscale modelling methodologies are performed in order to answer critical issues, reduce the time and cost of evaluating materials, understand phenomena not visible by one method alone, refined materials development, obtain a better lifetime prediction, and to reduce the time and cost of evaluating possible candidate materials. The collaborative EU programs aim to build the knowledge database in Europe as well as train and educate European researchers. Clearly it is necessary that the EU consortium of modellers and experimentalists continues to expand to address nuclear materials issues.

References

[1] <http://cordis.europa.eu/fp7/euratom/home_en.html>.
[2] <http://cordis.europa.eu/fp7/jrc/home_en.html>.

[3] <http://www.jet.efda.org/>.
[4] <http://www.iter.org/>.
[5] M. Samaras, W. Hoffelner, M. Victoria, J. Nucl. Mater. 371 (2007) 28.
[6] MRS Bulletin, 32(11) (2007).
[7] <http://cordis.europa.eu/data/PROJ_FP5/ACTIONeqDndSESSIONeq112182005-919ndDOCeq499ndTBLeqEN_PROJ.htm>.
[8] <ftp://ftp.cordis.europa.eu/pub/fp5-euratom/docs/vocalist_projrep_en.pdf>.
[9] <ftp://ftp.cordis.europa.eu/pub/fp6-euratom/docs/fisa2006_ws4_salome.pdf>.
[10] S. Jumel, J.C. Van Duysen, J. Ruste, C. Domain, J. Nucl. Mater. 346 (2005) 79.
[11] <www.nurresim.com>.
[12] R.C. Pasianot, L. Malerba, J. Nucl. Mater. 360 (2007) 118.
[13] C.S. Becquart, J.M. Raulot, G. Bencteux, C. Domain, M. Perez, S. Garruchet, H. Nguyen, Comput. Mater. Sci. 40 (2007) 119.
[14] C.S. Becquart, A. Souidi, C. Domain, M. Hou, L. Malerba, R.E. Stoller, J. Nucl. Mater. 351 (2006) 39.
[15] C.S. Becquart, Nucl. Instrum. and Meth. B 228 (2005) 111.
[16] M. Lambrecht, L. Malerba, A. Almazouzi, J. Nucl. Mater. (2008), doi:10.1016/j.jnucmat.2008.06.030.
[17] E. Vincent, C.S. Becquart, C. Pareige, P. Pareige, C. Domain, J. Nucl. Mater. 373 (2008) 387.
[18] B. Marini, J.P. Massoud, S. Bugat, D. Lidburry, ICFRM 2007, #521.
[19] M. Victoria, S. Dudarev, J.L. Boutard, E. Diegele, R. Lässer, A. Almazouzi, M.J. Caturla, C.C. Fu, J. Källne, L. Malerba, K. Nordlund, M. Perlado, M. Rieth, M. Samaras, R. Schaeublin, B.N. Singh, F. Willaime, Fus. Eng. Des. 82 (2007) 2413.
[20] C.C. Fu, F. Willaime, P. Ordejon, Phys. Rev. Lett. 92 (2004) 175503.
[21] P. Olsson, I.A. Abrikosov, L. Vitos, J. Wallenius, J. Nucl. Mater. 321 (2003) 48; P. Olsson, J. Wallenius, C. Domain, K. Nordlund, L. Malerba, Phys. Rev. B 72 (2005) 214119.
[22] D. Nguyen-Manh, A.P. Horsfield, S.L. Dudarev, Phys. Rev. B73 (2006) 020101.
[23] S. Dudarev, P.M. Derlet, J. Phys. Condens. Matter 17 (2005) 7097.
[24] C.C. Fu, J. Dalla Torre, F. Willaime, J.-L. Bocquet, A. Barbu, Nat. Mater. 4 (2005) 68.
[25] C. Ortiz et al., MRS Symposium Proceedings, 2005.
[26] M. Samaras et al., unpublished.
[27] R. Schaeublin, Y.L. Chiu, J. Nucl. Mater. 362 (2007) 152.
[28] <http://www.ciemat.es/recursos/doc/Redes_Cientifico_Tecnicas/VII_PM/180-430089_12200810481.pdf>; <http://www.efnudat.eu/FZD_workshop/Friday/1502_0910_Bhatnagar.pdf>.
[29] <www.fzd.de/db/Cms?pOid=27025>; C. Fazio, ANS Meeting, Anaheim, 2008.
[30] <http://www-ist.cea.fr/publicea/exl-doc/200700001902.doc>.
[31] <http://www.raphael-project.org/index.html>.
[32] <http://www.extremat.org/>.
[33] <http://www.snetp.eu/scripts/home/publigen/content/templates/show.asp?L=EN&P=114&vTicker=alleza&ITEMID=3>.
[34] <http://ec.europa.eu/energy/nuclear/forum/bratislava_prague/2007_11_26/index_en.htm>.
[35] <http://www.hy-co-era.net/datapool/page/8/050318_FROISBHFP.pdf>; <ftp://ftp.cordis.europa.eu/pub/fp7/docs/euratom-fission_ev20070921_vision-report_en.pdf>.
[36] M. Samaras, W. Hoffelner, C.-C. Fu, M. Guttmann, R.E. Stoller, in: Proceedings of ICAPP 2007, also published in Revue Générale Nucléaire, SFEN, France.
[37] <http://www.nea.fr/html/science/wpmm/index.html>.
[38] <http://www-naweb.iaea.org/napc/physics/meetings/TM34567.html>.
[39] <http://www.euronuclear.org/aboutus/yg/young.htm>.
[40] <http://www.iync.org/>.