EFDA WORKPROGRAMME 2010

Call for Participation

Emerging Technologies
Fusion Materials Topical Group

Research Project:
MAT-REMEV: Radiation Effects Modelling and Experimental Validation

Index

1. Introduction

At its meeting in Barcelona on the 8th of July 2009, the EFDA Steering Committee approved the EFDA 2010 Workprogramme, including the tasks identified below. This Call for Participation covers the activities for the 2010-WP of the MAT-REMEV Research Project of the Fusion Materials Topical Group, Radiation Effects Modelling and Experimental Validation, and will be implemented on the basis of the provisions given in Art. 5 of EFDA Agreement.

2. Objectives

The modelling activities under the Fusion Materials Topical Group pursue two objectives of (i) supporting Fusion for Energy (F4E) with the research project MAT-REMEV: Radiation Effects Modelling and Experimental Validation, and (ii) progressing with the development of materials for the possible use in DEMO. With respect to the first objective, the programme is focused, as a matter of priority, on the development of quantitative numerical tools for quantitative modelling and inter-correlating the radiation effects in EUROFER associated with its exposure to neutrons of various energy spectra. The validated tools and the associated experimental database will provide the basis for the optimisation of the IFMIF programme and for the assessment & extrapolation of the available data to the entire range of operational conditions encountered in DEMO for a reliable licensing process. The present document describes this first set of activities. The activities related to the second objective, namely modelling to support the development of ODS ferritic steels and of tungsten / tungsten alloys, are integrated in the corresponding research project work programme.

The objectives of the 2010 Work Programme of MAT-REMEV are defined according to the Strategic Objectives for Fusion Materials Modelling and Experimental Validation (2010-2015) [1] and in continuity with the achievements of WP-2008-2009. The main 2010-WP objectives are given below following the classification of Strategic Objectives 2010-2015 [1]:

(i) Cohesion

This activity encompasses the development of statistical methods to calculate the Gibbs free energy based on the energy of a limited set of atomic configurations calculated *ab initio* at 0 K. The development & first parameterisation of Spin Lattice Dynamics (SLD), in semi-classical atomistic approach, will provide a physically based description of magnetic excitations (magnons) and lattice vibrations (phonons) and their coupling, required for predicting the free energies of the phases & relative stability of the Fe-Cr system, and describing the energies of radiation defects and the dynamics of defect production in high-energy collision cascades generated by fusion neutrons.

(ii) Phase Diagram and phase transformation kinetics of the Fe-Cr system

Phase stability of the Fe-Cr system is an essential topic, as the formation of chromium-rich α' precipitates triggers hardening and embrittlement of ferritic/martensitic steels under fission neutron irradiation. The 2010-WP is devoted to the *ab initio* calculation of the ground state energy of the σ-phase and the application of Magnetic Cluster Expansion (MCE) developed in the 2008-2009 WP to the prediction of stability of this phase under equilibrium conditions. In addition introducing ballistic replacements and point defects in the MCE will provide a first evaluation of the α' and σ-phase stability under irradiation.

(iii) Displacement cascades: the long-time scale evolution

The objective of this activity is, by using the best available Fe-Cr-C potentials, to evaluate the sensitivity of the long-time scale kinetics of the radiation induced microstructure to the initial configuration of defect

[1] http://www.efda.org/about_efda/activities-fusion_materials.htm

structures predicted by MD simulations. In this context microstructure means the distribution of clusters of defects and alloying elements (carbon and chromium) in crystalline matrix modelled by Atomic kinetic Monte Carlo (AkMC). The expected outcome of this activity is a model for long-term evolution of displacement cascades, capable of predicting the fraction of freely migrating defects, defect clusters, and their interaction with alloying elements.

(iv) He & H and damage accumulation

Although the reduced activation ferritic/martensitic steels (RAFMS) exhibit very low swelling under fission neutron irradiation, several results reported in the open literature indicate that they might swell significantly under triple ion beam irradiation (dpa=self-ion, He, H) at fusion relevant He/dpa and H/dpa ratios. The *ab-initio* calculations and the development of Object kinetic Monte Carlo (OkMC) initiated in the 2008-2009 WP will be continued to model the kinetics of He-H-V-C clustering in the Fe-Cr matrix (in solid solution or in the presence of chromium precipitates), close to grain boundaries and in the bulk, with a particular attention paid to the role played by H and C. An atomistic AkMC will also be parameterised for comparison with OkMC.

(v) Kinetics: Development of advanced methods.

Advanced kinetics methods are key issues for predicting radiation effects in complex, often concentrated alloys, under irradiation up to high doses and high contents of He and H, as it involves numerous species and events, and also long times. Two types of modelling are proposed to be developed. These are new important activities required to bring modelling in closer contact with experimental observations, specifically in terms of addressing the necessary long time scales and large system sizes.
The First Passage kinetic Monte Carlo (FPkMC) has been proposed and initially developed by the LLNL on the basis of the Event kinetic Monte Carlo (EkMC) investigated at CEA Saclay earlier. The latter was successfully used to predict the radiation damage recovery stages in pure α-Fe at the beginning of the Radiation Effects Modelling Programme. FPkMC in principle exhibits linear scaling as a function of the number of objects involved in a simulation, and in this way is well adapted to treat complex systems and long time scale kinetics. Predictions made by FPkMC will be compared to the kinetics of well characterized model systems, like pure iron, and then adapted and parameterised for the Fe-Cr system for the fusion relevant irradiation conditions, and compared with AkMC and OkMC predictions (see above).
Another development route is to use Mean Field coarse-grained modelling, where the treatment of diffusion is based on atomic scale predictions and the coarse graining procedure adapted for transferring information up from the atomic scale. This method will be developed for the Fe-Cr system, with diffusion mechanisms involving vacancies and interstitials, and assessed versus phase stability.

(vi) Plasticity and fracture

The slow dynamics of screw dislocations is the controlling mechanism for plasticity and the onset of brittle fracture of bcc metals and alloys, and hence this dynamics is the controlling factor for the Ductile Brittle Transition Temperature (DBTT). This requires that *ab-initio* calculation of dynamical properties and interaction of screw dislocations with chromium, carbon & helium be pursued.
Plasticity modelling at the meso-scale via Discrete Dislocation Dynamics also requires increased effort. The Green’s function formalism will be introduced, as it is required to describe the anisotropic elasticity typical of high temperature behaviour of α-Fe and ferritic/martensitic steels. This should result in the quantitative prediction for the effect of α-Fe and steel softening at high temperature close to the α-> γ transformation temperature.

(vii) Visco-plasticity

During normal operation, materials of the Tritium-Breeding Blankets and Divertor will be in the range of temperatures and stresses where thermal and/or irradiation creep represents the dominant long-term time-dependent deformation mechanism. Dislocation climb also has to be introduced in the DDD codes to predict the observed deformation rates occurring under irradiation. One of the objectives of the WP-2010 is to initiate this activity.

(viii) Experiments: development & user's facilities

A close link between experiment and modelling is essential for the experimental validation of numerical models. The pure α-Fe and Fe-Cr model alloys already produced on behalf of EFDA will be extensively used.
The effort to define experimental conditions for pre-implanting, and, subsequently carrying out thermal He desorption spectroscopy experiments will continue. In parallel, ion irradiation under multiple ion beam conditions will allow testing the kinetic models for He, H and dpa accumulation.

The effort to develop electrical resistivity measurements down to cryogenic temperatures after ion irradiations should result in 2011 in well assessed results after proton irradiation (penetration ~100 micrometers) and feasibility assessment after self ion irradiation (penetration depth ~a few micrometers).

The experimental techniques and methods that are expected to be used for validation of models, and for exploration of a range of timescales, temperatures, stress states, and irradiation conditions, include *in-situ* and *ex-situ* electron microscopy for the examination of defect and dislocation microstructures. Also they include atom probe tomography for examining nano-chemistry and precipitation effects in alloys and ion irradiated specimens, and the ion beam irradiation facilities themselves. It is expected that advantage should be taken of the closely related methods like electron energy loss spectroscopy for cross-validation of atom probe tomography studies, and numerical TEM image simulations. Mössbauer spectroscopy, synchrotron radiation based EXAFS and related methods, and neutron diffraction could bring extra capacity in validating theoretical models and predictions.

The activities (i)-(viii) described above, the main objectives, milestones, and deliverables, have been defined in collaboration with F4E, and are intended to support the F4E EUROFER programme. The summary of all the activities is given in table 1 below with the estimate of Human Resources and other expenditures, which amount to 23.5ppy and 705 k€ for 2010 Base Line Support.

3. Work Description and Breakdown

3.1 Work Breakdown

For every objective listed above Work Breakdown in terms of milestones and deliverables within the WP-2010 approved by the Steering Committee is given below.

(i) Cohesion

Objectives milestones and deliverables are given in the table hereafter.

(i) Cohesion		
Objectives	**Milestones**	**Deliverables**
Spin-Lattice Dynamics	Development of an electronic structure based spin-lattice dynamics model within a semi-classical atomistic approach.	**12/2010: Report on** a semi-classical atomistic approach of spin-lattice dynamics and its parameterisation.
Magnetic Properties, Mössbauer effect & Small Angle Neutron	Determination of Short Range Order (SRO), crystalline structure & magnetic properties	**12/2010: Report on** Short Range Order (SRO), crystalline structure & magnetic properties of Fe-Cr

Scattering (SANS) .	of Fe-Cr model alloys.	model alloys after various heat treatment.

(ii) Phase Diagram and phase transformation kinetics of the Fe-Cr system.

Objectives milestones and deliverables are given in the table hereafter.

(ii) Phase Diagram and phase transformation kinetics of the Fe-Cr system		
Objectives	**Milestones**	**Deliverables**
First Principles modelling of precipitation of σ-phase in Fe-Cr model alloys.	Transformation path (displacement + rotation) & step energies from the bcc Fe-Cr to the σ-phase for several Cr contents.	**12/2010: Report on** the cohesive energy of σ-phase as deduced using the two step transformation from the bcc Fe-Cr for several Cr contents.
Magnetic Cluster Expansion (MCE).	Development of MCE including vacancies and Self Interstitial Atoms.	**12/2010: Report on** vacancies and SIAs energies in Fe-Cr described on via MCE.

(iii) Displacement cascades: the long-time scale evolution

Objectives milestones and deliverables are given in the table hereafter.

(iii) Displacement cascades: the long-time scale evolution		
Objectives	**Milestones**	**Deliverables**
Displacement cascade simulation in Fe-Cr-C model alloys.	Development of interatomic potentials for Fe-Cr-C alloys & determination of cascade overlapping effects in Fe-Cr-C.	**12/2010: Report on** the new Fe-Cr-C potential and on cascade overlapping effects in FeCrC.

(iv) He & H and damage accumulation

Objectives milestones and deliverables are given in the table hereafter.

(iv) He & H and damage accumulation		
Objectives	**Milestones**	**Deliverables**
DFT calculations: (i) He H & C energetics near Grain-Boundaries (GB), (ii) role of Cr on the energetics of He, V & their clusters.	(i) Effect of C on the diffusion at GB compared to bulk, (ii) Migration energies of He & Cr in Fe-Cr model alloys at various Cr contents.	**12/2010: Report on** (i) Diffusion of He close to GB in presence of C (ii) He & V migration in Fe-Cr model alloys.
DFT based OKMC development: to predict the evolution of He and point-defects produced in Fe-Cr-C alloys with GB under irradiation.	First comparison of OKMC with dual beam induced microstructure in Fe-Cr model alloys (see activity viii). Identification of experiments for validating OKMC predictions, and initial comparison of model data with experimental results.	**12/2010: Report on** first comparison of OKMC model with experimental data obtained via ion-beam irradiation in JANNUS. Identification of model limitation & modifications
DFT based Atomic kinetic Monte Carlo (AkMC) including He within Fe-Cr alloys with GB under irradiation.	Implementation of He diffusion mechanism in bcc Fe in AkMC code. First computation on α/α' unmixing.	**12/2010: Report on** implementation of He diffusion mechanism in AkMC code. First AkMC simulation of α/α' unmixing.

(v) Kinetics: Development of advanced methods

Objectives milestones and deliverables are given in the table hereafter.

(v) Kinetics: Development of advanced methods		
Objectives	**Milestones**	**Deliverables**
Develop & validate a First Passage kinetics Monte Carlo (FPkMC) method	Implementation & validation of the FPkMC versus (i) Event kMC (EkMC) & experiments (Resistivity Recovery in UHP Fe), and, (ii) AkMC for well assessed dilute systems.	**12/2010: Report on** the implementation of First Passage kMC and benchmarking against experimental data & modelling tools such as EkMC & AkMC. Efficiency (N-method).
Develop a meso-scale kinetic code to simulate the diffusion transport in concentrated alloys under irradiation	Introducing vacancy diffusion mechanism into a Phase Field Model with fluctuations. Calculating the driving force as a function of temperature and concentration (solid solution & demixed Fe-Cr system).	**12/2010: Report on** the calculated driving forces in the Phase Field model in the case of a Solid solution and demixed binary alloy with vacancy-diffusion mechanism.
Atomic kinetic Monte Carlo (AkMC) coupled with Artificial Intelligence (AI).	Coupling kMC with AI & assessing the effect of the initial training set obtained from empirical potentials and DFT calculations.	**12/2010: Report on** AkMC unmixing of Fe-Cr system with migration barriers calculated via AI from an initial set based on empirical potential & DFT calculation. Effect of the initial set of data.

(vi) Plasticity and fracture

Objectives, milestones and deliverables are given in the table hereafter.

(vi) Plasticity and Fracture		
Objectives	**Milestones**	**Deliverables**
DFT calculations: energetics of screw & edge dislocations under stress in α-Fe with impurities.	DFT & empirical potential based calculation of the crystal orientation dependence of the Peierls stress & glide plane of straight dislocations. Methodological development using empirical potential concerning kink formation under stress.	**12/2010: Report on Methodological developments using empirical potentials & DFT**: (i) 1/2<111> dislocation kink formation under stress, (ii) kink formation enthalpy in {211} planes, (iii) core structure & Peierls barrier of <100> screw, 1/2<111> edge & mixed dislocations.
Experimental validation of dislocation dynamics properties	In-situ TEM observation of dynamics of screw & edge dislocation in binary Fe-Cr model-alloys versus temperature. High strain rate tensile testing of pure α-Fe.	**12/2010: Report on** (i) Cr effect on dynamics of screw dislocation. Comparison with DFT prediction. (ii) High strain rate tensile testing of pure α-Fe. Comparison with MD simulation.
Screw dislocation mobility in presence of nanometric obstacles observed in TEM. Micromechanical testing of Fe model alloy	TEM observation of mobility of screw dislocation in the presence of nanometre-size obstacles introduced by ion-beam irradiation. The determination of dislocation mobility laws from TEM observations. Side effect and glide plain identification in micromechanical testing; effects of grain boundaries and C and Cr.	**12/2010: Report on** TEM observation of screw dislocation mobility in presence of nanometre-size obstacles. MD simulation of observations. Comparison with dislocation mobility laws determined by TEM observation. 12/2010: Report on micromechanical test and interpretation
MD simulations: (i) hardening due to radiation induced defect clusters and (ii) effect of carbon on the mobility of dislocation loops and vacancy clusters.	Reaction mechanisms of 1/2<111> screw dislocation with 1/2 <111> & <100> dislocation loops. Interaction of 1/2<111> screw dislocation with Cr precipitates. Effect of C on the energy & mobility of V & SIA clusters	**12/2010: Report on** (i) interaction mechanisms of 1/2<111> with dislocation loops and Cr-precipitates and (ii) effect of C on the mobility of vacancies and SIA clusters.
3D Discrete Dislocation Dynamics within anisotropic elasticity theory.	DDD code with anisotropic elasticity of α-Fe including temperature dependence of the elastic stiffness constant.	**12/2010: Report on** calculated 3-D dislocation microstructure and prediction of yield strength softening versus temperature in α-Fe.

(vii) Visco-plasticity

Objectives milestones and deliverables are given in the table hereafter.

(vii) Visco-plasticity		
Objectives	**Milestones**	**Deliverables**
DDD model including dislocation climb under irradiation	Dislocation climb model with vacancy pipe-diffusion & vacancy-jog interaction.	**12/2010: Report on** DD simulations of dislocation climb controlled by V diffusion.

(viii) Experiments: development & user's facilities

Milestones and deliverables are given in the table hereafter.

Experiments: development & user's facilities		
Objectives	**Milestones**	**Deliverables**
Kinetic Modelling validation: Mono & dual beam irradiation in JANNUS followed by TEM & TAP characterisation of the microstructure.	TEM characterisation of Fe and Fe-Cr alloys under self-ion irradiation (dpa) and self-ion & He implantation.	**12/2010: Report on** TEM characterisation of Fe and Fe-Cr alloys under self-ion and self-ion & He implantation
He-diffusion mechanisms validation: thermal He-desorption spectroscopy.	He-desorption on pre-implanted a-Fe and Fe-Cr model alloys in conditions determined by modelling	**12/2010: Report on** comparison of experimental desorption spectroscopy & modelling prediction for a-Fe & Fe-Cr model-alloys
Primary damage in pure α-Fe & Fe-Cr alloys: identification of dislocation loops and He bubbles.	Characterisation of radiation damage and He bubbles in pure Fe and Fe(C, Cr) model alloys, assisted by TEM image and EELS process simulation.	**12/2010: Interim report on** radiation damage in and He bubbles in pure Fe and Fe(C, Cr) model alloys.
Technical feasibility of experimental set-ups for electrical resistivity measurements at cryogenic temperature on discs of a few micrometers thickness.	(i) Completion of electrical resistivity measurements at cryogenic temperature on Fe-Cr sample of ~100 micrometers thickness, (ii) First elements of feasibility study on specimens of a few micrometers thickness, (iii) Investigation of resistivity recovery of cold-worked high purity irradiated specimens, including the comparison of electron- and ion-irradiated specimens.	**12/2010: Report on** evaluation of the set-up devoted to electrical resistivity measurement on ~100 micrometer thick Fe-Cr specimens. The report should desirably include also the investigation of resistivity recovery of cold-worked high purity irradiated specimens, including the comparison of electron- and ion-irradiated specimens.
Quantitative TEM &SEM examination of EUROFER irradiated	Completion of quantitative TEM & SEM investigation on EUROFER irradiated in SPICE,	**12/2010: Report on** TEM & SEM examined microstructure in EUROFER irradiated in

in SPICE (15 dpa), WTZ (15 dpa) and Arbor1 (30 dpa).	WTZ & ARBOR1.	SPICE, WTZ and ARBOR1. Comparison with the modelling prediction.

(ix) Priority support

Quantitative prediction of behaviour of the Fe-Cr-C system (model-EUROFER) under fusion relevant reactor conditions is a realistic objective provided that (i) the adequate physically based methods are developed and parameterised using presently available high-accuracy *ab-initio* calculations, and, (ii) the experimental validation is adequately linked to the theoretical and numerical predictions.

Given the need for a special effort of experienced scientists having a unique expertise in modelling concerning *ab initio*, innovative methods such as the treatment of magnetic-lattice effects in Fe-Cr alloys responsible for variation of mechanical properties, advanced kinetic tools, DDD treatment of plasticity and experimental validation implying ion-beam irradiation and He-desorption spectrometry directly linked to modelling, **the following part of the total effort is proposed to be funded under Priority Support**.

Priority Support for 2010:

The expenditure concerns development of ground-breaking advanced tools and a collaborative effort foreseen to involve several Associated Laboratories centred on the use of a dual beam facility for testing and validating of models through the investigation of microstructure up to high doses and He (& H) contents, and of He-desorption experiments under conditions guided by modelling. The cost encompasses the operation of the facilities, the mounting, follow-up and dismounting the experiments. The estimation of the costs is based on 120 hours of operation of a dual beam facility and 600 hours of He-desorption spectroscopy facility.

Overall resources proposed under P.S.: 6.75 PPY and 160 k€ (details in table 2 hereafter).

Table 2: WP-2010: Human Resources and Expenditures proposed for Priority Support

2010 Priority Support	**PPY**	**Expenditure**	**Comments**
Coordination	0.5		0.4PPY +0.1 TPY
Spin-Lattice Dynamics Development	0.5		
σ-phase stability and MCE including point defects	0.5		
Empirical Potential & Collision cascades in Fe-Cr-C. Investigation of sensitivity to the initial conditions	1.0		
Ab-initio energetic of He-V-C and He-V-Cr in the bulk and grain-boundaries (GB)	0.5		
Development of OKMC for He & dpa in bulk & GB based on *ab-initio*	0.5		
Ab-initio energies of screw dislocation & double kink	0.5		
In-situ electron microscope (TEM) observations to validate the predicted dislocation mobility laws and models for interaction of dislocations with nanometre-size obstacles. Observation of microstructural changes associated with	0.75		

resistivity recovery stages.			
Kinetics: advanced method development	0.5		
Resistivity recovery measurements at cryogenic temperatures, comparison of electron- and ion-irradiated specimens. Possible extension to the case of cold-worked samples.	0.25		
Experimental validation of He OKMC kinetics via He desorption and dual/beam induced microstructure characterisation	0.75	160	Facility Operation: (i) 40 k€ for He desorption and (ii) 120 k€ for dual beam up to high dose and He content
Measurements of the magnetic properties of the Fe-Cr system versus temperature.	0.5		
Total 2010 Priority Support	**6.75**	**160**	

3.2 JET related activities

Non applicable.

3.3 Publications

A list of publications produced on the basis of results of the 2010-WP, will be compiled after the completion of these tasks.

4. Scientific and Technical Reports

4.1 Progress reports

At the end of each calendar year and at intermediate times where appropriate, the Task Coordinator shall submit a report on activities under the Task Agreement to the EFDA Leader for his approval. These reports shall describe the progress made by each Association on each activity, and they shall indicate the level of achievement of the objectives, the status of the activities, the allocation of resources and recommendations for the next year where applicable. The EURATOM financial contribution will be made through the usual procedures for baseline support through the Contract of Association.

4.2 Report of achievements under Priority Support (final report and, when appropriate, intermediate reports):

The progress of tasks undertaken under Priority Support and the status of deliverables will be reported separately to the EFDA Leader. A final report (and intermediate reports indicating any substantial progress in the achievement of deliverables, if requested by the EFDA Leader) shall be prepared by the Task Coordinator and submitted to the EFDA Leader. These reports shall include specific sub-sections for each of the Associations involved. They shall document the degree to which the deliverables outlined have been achieved, and shall include a breakdown of expenditure for each Association. The EURATOM financial contribution will be made after approval by the EFDA Leader of these reports.

4.3 Milestones.

The results obtained within the Research Radiation Effects Modelling and Experimental Validation will be presented by the principal investigators and reviewed during joint monitoring meetings held twice a year. On this basis the progress accomplished by the contributing Associations will be reported by the Coordinator to the EFDA Leader.

The report on the Association activities under Priority Support will be prepared by the Coordinator to be presented to the EFDA Leader at the end of every calendar year.

The final and technical report will be submitted to the Responsible Officer of the Topical Group for approval and uploading the IDM database.

5. Association Proposal

The Associations are requested to complete the Association Response via ECoM system.