EFDA WORKPROGRAMME 2011

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 Dublin on the 23rd June 2010 the EFDA Steering Committee approved the EFDA 2011 Workprogramme, including the tasks identified below. This Call for Participation covers the activities of the 2011-WP of the MAT-REMEV Research Project of the Fusion Materials Topical Group on **Radiation Effects Modelling and Experimental Validation (REMEV)**, and will be implemented on the basis of the provisions given in Art. 5 of the EFDA Agreement.

2. Objectives

Presently there is still no direct means for obtaining reliable quantitative information, required for engineering design studies, about changes of physical and mechanical properties, and about the nature of potential breakdown modes of structural and plasma-facing materials resulting from fusion neutron irradiation and thermal loading in DEMO. Operation of the present generation of fusion devices including JET, Tore-Supra, and Asdex Upgrade has already highlighted a range of generic materials-science-related problems not foreseen in the past, for example materials compatibility in the divertor, or the fact that a substantial amount of tritium is retained in the plasma-facing materials. There is an evident need to develop capabilities for identifying the principal fundamental causes of degradation of materials in DEMO environment, and understanding changes in the properties of materials occurring under fusion neutron irradiation.

The programme of activities outlined below is based on the extrapolation of recent advances in modelling and experimental validation techniques (including information obtained using fission reactor irradiation experiments). The experimental irradiation and testing methods, which recently proved effective when applied in combination with quantitative modelling of materials, include ion-beam irradiation experiments, micromechanical tests, and *in-situ* electron microscopy.

The central objective of REMEV research project is the further development of the conceptual and quantitative framework for the interpretation of results of experimental tests on steels, iron-based alloys, and several other types of candidate structural materials, and predicting the performance of these materials under DEMO-relevant operating conditions.

The structure MAT-REMEV research project is based on the established principles of multi-scale mathematical modelling of materials, which are applied to steels, iron-based alloys, and several other types of candidate structural materials, and focuses on:

- Interatomic bonding and phase stability.
  Priority issues: modelling irradiation-driven α′ precipitation, mixing of high-Cr alloys by irradiation, effect of carbon on defects, and high-temperature properties of steels.
- Radiation damage accumulation and evolution of microstructure.
  Priority issues: accumulation of helium at grain boundaries and the evolution of defect and dislocation network under irradiation and thermal recovery.
- Deformation and plasticity.
  Priority issues: modelling high-temperature deformation and fracture, radiation hardening and embrittlement, including the effects of α′ precipitation.
- Experimental validation of models.

Priority issues: dual/triple ion beam irradiation and *in-situ* electron microscope examination of microstructure, thermal recovery tests, helium migration analysis, atom probe tomography of irradiated model alloys and steels.

The main objective of these activities is the development of rational quantitative scientific understanding of changes in mechanical properties of steels and several other types of structural fusion materials occurring under DEMO-relevant operating conditions.

The modelling methods and the corresponding experimental database will provide a basis for the optimisation of the IFMIF programme and for the assessment and extrapolation of data to the operating conditions in DEMO for licensing purposes. Activities related to modelling tungsten and tungsten alloys are integrated in a separate research project of the same Work Programme.

The objectives of the 2011 Work Programme of MAT-REMEV are defined according to the Strategic Objectives for Fusion Materials Modelling and Experimental Validation (2010-2015) [1] and are the continuation of the work done within WP-2008-2009-2010.

3. Work Description and Breakdown

3.1 Work Breakdown

Interatomic bonding and phase stability. This activity includes *ab initio* investigation of small defects formed by irradiation and dislocations, the development of *ab initio*-based interatomic potentials for molecular dynamics simulations, including spin-lattice dynamics simulations of high temperature properties of magnetic iron-based alloys, the development of Monte Carlo methods for modelling equilibrium phase diagram and phase stability under irradiation, the kinetics of α′ precipitation and evolution of carbon-related microstructures, and phase decomposition of alloys under irradiation. The analysis of phase stability of model alloys has now been extended to Fe-Cr-C steels, and new tasks have been launched, aimed at assessing the radiation stability of ODS alloys. The activity also includes a task on *ab initio* modelling of radiation damage effects in beryllium.

Objectives	**Milestones**	**Deliverables**
High-temperature properties of iron	Development of a model for high temperature elastic properties of iron, based on spin lattice dynamics.	**12/2011: Report on** Atomistic simulation of high temperature elastic properties of iron and the parameterization of the spin-lattice dynamics model.
α′ precipitation and radiation defect accumulation in Fe-Cr model alloys	Determination of rates of Cr precipitation, investigation of SRO and magnetic SRO, and assessment of rates of radiation mixing and defect accumulation in the matrix and in precipitates in Fe-Cr model alloys.	**12/2011: Report on:** Determination of rates of Cr precipitation, investigation of SRO and magnetic SRO, and assessment of rates of radiation mixing and defect accumulation in the matrix and in precipitates in Fe-Cr model alloys.

Structure and cohesion of grain boundaries in iron and Fe-Cr alloys.	Structure and cohesive energies of grain boundaries in Fe and Fe-Cr alloys by *ab initio*. Accumulation of helium, GB de-cohesion.	**12/2011: Report on:** Structure and cohesive energies of grain boundaries in Fe and Fe-Cr alloys by *ab initio*, and helium-driven decohesion of GBs. Comparison of DFT results with MD simulations.
Grain boundary structure and statistical distribution of grain boundary types in iron.	Structures and cohesive energies of grain boundaries in pure iron predicted by atomistic simulations, including finite temperature effects and the presence of vacancies.	**12/2011: Report on:** Simulated grain boundary structures in pure iron predicted by atomistic simulations, including finite temperature effects and the presence of vacancies.
Segregation of Cr to grain boundaries and dislocation loops.	Determination of equilibrium structures of grain boundaries and dislocation structures in Fe-Cr alloys, Cr segregation.	**12/2011: Report on: The** determination of equilibrium structures of grain boundaries and dislocation structures in Fe-Cr alloys, including the analysis of Cr segregation effects.
Structure of radiation defects and dislocation in beryllium	Develop an *ab initio* model for radiation defect structures and defect migration pathways in beryllium.	**12/2011: Report on:** An *ab initio* model for radiation defect structures and defect migration pathways in beryllium.
Cohesion and structure of the σ phase in Fe-V alloys.	Develop a model for the σ phase of iron-vanadium alloys	**12/2011: Report on: A** model for the free energy of the σ phase of iron-vanadium alloys.
Cohesion and structure of the σ phase in Fe-Cr alloys.	Develop an *ab initio* model for the σ phase in Fe – Cr alloys.	**12/2011: Report on:** *Ab initio* model for the σ phase in Fe – Cr alloys.
Atom probe tomography of ion-irradiated model alloys.	Using atom probe tomography, investigate the dose, dose rate and composition dependent phase decomposition of Fe-Cr alloys under ion irradiation.	**12/2011: Report on:** Atom probe tomography investigation of the dose, dose rate and composition dependence of phase decomposition of Fe-Cr alloys resulting from ion irradiation.
Structure of screw and mixed dislocations in Fe, including double kink configurations.	Develop an *ab initio* model for screw and mixed dislocations in Fe and investigate double kink structures and energies.	**12/2011: Report on:** *Ab initio* model for screw and mixed dislocations in Fe, and double kink structures and energies.
Stability and kinetics of alloying elements in ODS materials	a) Determination of cohesive energies, and barriers for migration of yttrium, titanium and oxygen complexes in Fe-Cr alloys, and energies of formation of mixed Ti-Y oxides in Fe-Cr matrix. b) First-principles evaluation of interaction of yttrium, titanium and oxygen with vacancies.	**12/2011: Report on:** a) Determination of cohesive energies, and kinetic barriers for migration of yttrium, titanium and oxygen in Fe-Cr alloys, and energies of formation of mixed Ti-Y oxides in the Fe-Cr matrix. b) First-principles evaluation of interaction of yttrium, titanium and oxygen with vacancies.

Radiation damage accumulation and evolution of microstructure. This activity includes *ab initio* investigation of energies determining the kinetics of helium accumulation in steels, involving the investigation of irradiation-driven α′ precipitation and the role of carbon, modelling the structure and cohesion at grain boundaries (by *ab initio* and molecular dynamics methods), including effects of helium accumulation at grain boundaries. The

activity will also include the development of kinetic Monte Carlo, or similar, statistical methods, coupled with dislocation dynamics based methods for modelling radiation-induced microstructures, including modelling of thermal recovery (*ex-* and *in-situ*) of those microstructures.

Objectives	**Milestones**	**Deliverables**
Interaction of carbon with radiation defects and dislocations in pure Fe.	a) Perform first principles calculations and parameterize interaction of carbon with defects and dislocations in Fe b) Perform molecular dynamics simulations describing the interaction of carbon with radiation defects, defect clusters, and dislocations.	**12/2011: Report on:** First principles calculations and parameterization of interaction of carbon with defects and dislocations in Fe. **12/2011: Report on:** Molecular dynamics simulations describing the interaction of carbon with radiation defects, defect clusters, and dislocations.
Grain boundary segregation effects and GB de-cohesion due to helium accumulation.	Perform *ab initio* calculations to assess the combined effect of carbon, chromium and helium segregation on the strength of representative grain boundaries in pure Fe and Fe-Cr alloys.	**12/2011: Report on:** *Ab initio* calculations assessing the combined effect of C, Cr and He segregation on the strength of representative grain boundaries in pure Fe and Fe-Cr alloys.
Development of an object kinetic Monte Carlo code for radiation damage.	Formulate a code development strategy and implement it as a general purpose modular object kinetic Monte Carlo code for simulating radiation damage accumulation in complex materials.	**12/2011: Report on: A** code development strategy and implementation in the form of a general purpose modular object kinetic Monte Carlo code for simulating radiation damage accumulation in materials.
Development of an accelerated first passage Monte Carlo simulation code	Formulate and implement an accelerated FP Monte Carlo simulation code, benchmark predictions against existing codes.	**12/2011: Report on:** Formulation and implementation of an accelerated FP Monte Carlo simulation code, including benchmarking against the existing MC codes.
Synergetic effect of He, H, and self-ion irradiation on swelling.	Formulate a RT model for the synergetic effect of He, H and self-ion irradiation on the swelling of materials under irradiation.	**12/2011: Report on:** A RT model for the synergetic effect of He, H and self-ion irradiation on the swelling of materials under irradiation.
Phase stability and kinetics of solutes and radiation defects in dilute Fe-Cr-C alloys.	Perform *ab initio* calculations and AKMC modelling to assess the effect of carbon on the phase stability and kinetics of migration of solute atoms and radiation defects in Fe-Cr-C alloys.	**12/2011: Report on:** *Ab initio* and AKMC investigation of effects of carbon on the phase stability and kinetics of migration of solute atoms and radiation defects in Fe-Cr-C alloys.
Accumulation of radiation damage in Fe-Cr-C alloys.	Perform molecular dynamics simulations of collision cascades in Fe-Cr-C alloys, assess the effect of carbon the formation of radiation defects.	**12/2011: Report on:** Results of simulations of collision cascades in Fe-Cr-C alloys, including the assessment of the effect of carbon on the formation of radiation defects.

Alternative materials concepts. This activity, focused on the investigation of possible alternative materials for structural applications, includes a preliminary assessment of vanadium based alloys as *non-magnetic* candidate structural materials, and analysis of advantages and disadvantages associated with the use of vanadium alloys in fusion.

Objectives	**Milestones**	**Deliverables**
Assessment of physical properties of vanadium alloys.	Assessment of mechanical and physical properties of vanadium alloys and possible application of vanadium alloys as fusion structural materials.	**12/2011: Report on:** Assessment of mechanical and physical properties of vanadium alloys and possible application of vanadium alloys as fusion structural materials.

Deformation and plasticity. This activity includes the development of mathematical models for radiation hardening and embrittlement of fusion materials, rationalizing experimental observations on deformation and fracture, and the effect of α´ precipitation on the fracture properties of Fe-Cr based ferritic-martensitic and ferritic steels.

Objectives	**Milestones**	**Deliverables**
Radiation hardening of Fe-Cr alloys	Assessment of hardening effect of radiation defects and α´ precipitates.	**12/2011: Report on:** Quantitative assessment of hardening effect of radiation defects and α´ precipitates, and comparison with experimental observations.
High temperature loss of strength of iron and steels.	Identification of dislocation reactions responsible for the high temperature loss of mechanical strength of iron and steels.	**12/2011: Report on:** Dislocation reactions and microscopic model for the high temperature loss of mechanical strength of iron and steels.
Radiation embrittlement of iron and steels.	Evaluation of double kink energies for screw dislocations in iron and other bcc metals, using empirical potentials, including the effect of radiation defects.	**12/2011: Report on:** Evaluation of double kink energies for screw dislocations in iron and other bcc metals, using empirical potentials, including the effect of radiation defects.

Experimental validation of models. This activity includes the fabrication of dedicated model alloys and pure metals, irradiation experiments, and mechanical and microstructural examination of these materials. Experimental investigations will also include the analysis of evolution of helium microstructures, thermal recovery of electrical resistivity and radiation damage induced microstructures, performed both in *ex-* and *in-situ* modes, and changes in micro-magnetic properties under irradiation.

Objectives	**Milestones**	**Deliverables**
Fabrication of dedicated Fe-Cr model alloys	Fabrication of Fe-(3%, 8%, 12%, 18%, 25%) Cr high purity model alloys	**12/2011: Report on:** Fabrication of Fe-(3%, 8%, 12%, 18%, 25%) Cr high purity model alloys

TEM investigation of defects in neutron irradiated, and boron-doped EUROFER97.	TEM investigation of types, sizes and concentration of radiation defects in neutron irradiated and boron-doped EUROFER97.	**12/2011: Report on:** TEM experimental investigation of types, sizes and concentration of radiation defects in neutron irradiated and boron-doped EUROFER97.
Voids, helium bubbles, and α´ precipitates in neutron-irradiated steels.	Microstructural characterization of voids, helium bubbles and α´ precipitates in steels irradiated to 15 to 32 dpa.	**12/2011: Report on:** Microstructural characterization of voids, helium bubbles, and α´ precipitates in steels irradiated to 15 to 32 dpa.
In-situ defect dynamics in Fe-Cr alloys.	*In-situ* analysis of evolution of defect microstructures in Fe-Cr alloys, including surface effects and effect of Cr on mobility of defects	**12/2011: Report on:** *In-situ* analysis of evolution of defect microstructures in Fe-Cr alloys, including surface effects and effect of Cr on mobility of defects.
Short-range order in irradiated Fe-Cr alloys	a) Mössbauer spectroscopy determination of short-range order in irradiated Fe-Cr alloys. b) Neutron scattering investigation of de-mixing of Fe-Cr alloys. Analysis of magnetic short-range order in Fe-Cr alloys.	**12/2011: Report on:** a) Application of Mössbauer spectroscopy to the determination of short-range order in irradiated Fe-Cr alloys. b) Neutron scattering investigation of de-mixing of Fe-Cr alloys. Analysis of magnetic short-range order in Fe-Cr alloys.
Dose rate effects and comparison of neutron, ion-irradiation induced microstructures	Perform comparison of ion and neutron irradiation induced microstructures, identify and quantify the dose rate effects	**12/2011: Report on:** Comparison of ion and neutron irradiation induced microstructures, and identification and quantification of the dose rate effects.
Strain rate effect on microstructure of irradiated Fe and Fe-Cr alloys.	Perform irradiation tests and characterize microstructure of irradiated pure Fe and Fe-Cr alloys.	**12/2011: Report on:** Irradiation tests and characterization of microstructure of irradiated pure Fe and Fe-Cr alloys.
Rate theory model for resistivity recovery in Fe-Cr alloys.	Develop a RT model taking into account correlated pair recombination effects, and interpret resistivity recovery curves for Fe-Cr alloys.	**12/2011: Report on:** RT model taking into account correlated pair recombination effects, and interpret resistivity recovery curves for Fe-Cr alloys.
Magnetic properties and radiation damage recovery curves for Fe-Cr alloys.	Experimental observation and comparison with modelling predictions of magnetic properties and resistivity recovery curves for Fe-Cr alloys.	**12/2011: Report on:** Experimental observation and comparison with modelling predictions of magnetic properties and resistivity recovery curves for Fe-Cr alloys.
Benchmarking of RT model for helium desorption spectra against experimental data.	Develop a RT model for helium desorption from Fe including the treatment of carbon effects, and benchmark against TD experimental data.	**12/2011: Report on:** RT model for helium desorption from iron, including the treatment of carbon effects, and benchmarking the model against TD experimental data.
Determination of steady state operating temperatures for steels	Using neutron irradiation data and modelling, assess the operating temperature for steels giving rise to no irradiation embrittlement. Discuss the dose	**12/2011: Report on:** Assessment, using neutron irradiation data and modelling, of operating temperatures for steels giving rise to no irradiation

	rate effects.	embrittlement.

(i) Priority support

The estimated resources for 2011 for the MAT- REMEV research project are 6.75ppy and 180 k€ under Priority Support

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

2010 Priority Support	PPY	Expenditure	Comments
Coordination	0.5		
α´ precipitation and radiation defect accumulation in Fe-Cr model alloys	0.4		
Grain boundary segregation effects and GB de-cohesion due to helium accumulation.	0.5		
Synergetic effect of He, H, and self-ion irradiation on swelling	0.5		
Accumulation of radiation damage in Fe-Cr-C alloys.	0.5		
Radiation hardening of Fe-Cr alloys	0.4		
High temperature loss of strength of iron and steels.	0.4		
Radiation embrittlement of iron and steels.	1.0		
Fabrication of dedicated Fe-Cr model alloys	1.0	0	
Benchmarking of RT model for helium desorption spectra against experimental data.	0.3	20	
Dose rate effects and comparison of ion irradiation and neutron irradiation data	0.5		
Dual/ Triple ion bean irradiation and in – situ electron microscope examination of microstructure.	0.75	160	
Total 2010 Priority Support	**6.75**	**180**	

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 the ECoM system.

6. Bibliography

[1] J.-L. Boutard, M.J. Caturla, S.L. Dudarev, F. Willaime, Strategic Objectives for Radiation Effects Modelling and Experimental Validation 2010-2015, EFDA-D-2D4B78