EFDA Workprogramme 2013

Call for Participation

Materials R&D

Deadline for Responses: 17. Jan 2013

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This Call for Participation aims to implement the Materials R&D Workprogramme 2013 under Task Agreements as foreseen in the new EFDA Art. 5

Introduction

At its 52th meeting in Marseille on 3-4 October 2012, the EFDA Steering Committee approved the EFDA 2013 Workprogramme, including the tasks identified below. This Call covers the activities of the Area of Fusion Materials in the PPPT WP 2013 and will be implemented on the basis of the provisions given in Art.5 of the EFDA Agreement.

Programmatic Background

The development of fusion power generation concept into a commercially viable technology is the problem of optimization and balancing the factors that determine the availability of a fusion power plant against construction and operation costs. The cost of a fusion electricity unit increases both in the limit of large reactor size, due to the high level of investment required at the construction stage *and* in the limit of small reactor size due to the high running costs associated with the need to frequently replace components as well as due to the constraints imposed by the physics laws determining the behaviour of fusion plasma.

Whether the optimum design configuration corresponding to the minimum fusion electricity unit cost – found by optimizing the design for a given set of materials – proves economically viable, depends entirely on the selection of materials. The task of global design-materials optimization involves discovering innovative materials solutions that need to be formulated, developed, tested and manufactured specifically to match the needs of fusion power generation technology. One of the central objectives of the fusion materials programme is to identify innovative materials development routes, using scientific understanding and knowledge of how materials properties evolve and change in the operating environment of a fusion power plant.

1. MAT-HHFM:

Task Agreement WP13-MAT-HHFM:
High Heat Flux Materials

1.1 Introduction

At its 52th meeting in Marseille on 3-4 October 2012, the EFDA Steering Committee approved the EFDA 2013 Workprogramme. This Technical Specifications corresponds to the activities of the 2013-WP of MAT-HHFM Research Project on High Heat Flux Materials (HHFM) of the Fusion Materials Topical Group in the PPPT WP 2013. It will be implemented on the basis of the provisions given in Art. 5 of EFDA Agreement.

1.2 Objectives

The use of High Heat Flux materials, for different temperature cooling divertor concepts (Low/High) and possibly for the protection of the first wall in reactor designs beyond ITER is being investigated in this programme. The main objective is still to develop and demonstrate possible applications as well as to identify limitations for the use of this kind of materials in future fusion reactors. These will certainly differ significantly from ITER (i.e, much higher neutron irradiation dose and transmutation rates). But even neglecting irradiation effects (due to large gaps in the database), there are still unsolved problems related to the use and properties of tungsten materials.

The Work Programme 2013 is focused on the recommendations given in the European Fusion Roadmap, and in the Assessment of the EU R&D Programme on DEMO Structural and High-Heat Flux Materials group, addressing the following issues:

<u>W as divertor armour material</u>

- Intrinsic brittleness of W and further embrittlement due to irradiation and/or recrystallization
- Joining to underlying cooling structure, e.g. W to Cu or steel
- Determination/use of thermal shock and thermal fatigue limits/data (as input for materials development and optimization

<u>W as FW armour material</u>

- Oxidation (accident scenario, air ingress, sublimation and release of radioactive isotopes)
- Intrinsic brittleness of W and further embrittlement due to irradiation and/or recrystallization
- Coating process (W layer on EUROFER)
- Determination/use of thermal shock and thermal fatigue limits/data (as input for materials development and optimization)

<u>W as divertor structural material</u>

- Intrinsic brittleness of W and further embrittlement due to irradiation
- Joining W to steel (e.g. pipe-to-pipe)
- Materials database (un-irrad.)

Cu composites as divertor structural material (pipes)

- Development of Cu- based composite materials
- Database of engineering parameters of CuCrZr and GlidCop in the range of 100-350°C

1.3 Work Description and Breakdown

Structure

The programme is organized along five activities:

WP13-MAT-HHFM-01

Armour materials

This activity is dedicated to the study of Divertor shield, Blanket (First Wall) Protection, and specific qualification and characterization of armour materials. W alloys produced by mechanical alloying, PIM/MIM and powder chemistry will be considered for the divertor. For the blanket armour, self – passivation W alloys, W coating of EUROFER, functional gradient layers and special steels are the main lines of the programme. Special qualification and characterization cover thermal shock, thermal fatigue, H/He Beam loads, and standard properties (tensile, LCF, etc…) experiments.

Divertor shield

- Fabrication of material: verification of the effect of TiC addition; and improving the fabrication capacity.

Blanket (FW) protection

- Self-passivating alloys: production of larger amounts and characterization by intensive material tests
- Coating of EUROFER by tungsten. The investigation of appropriate processes and the evaluation of functional gradient layers

Specific qualification and characterization

- Characterization by e-beam (JUDITH facilities) and H/He beam load (GLADIS) as well as all available high temperature mechanical tests.

Main objectives include:

- Fabrication of a variety of different armour prototype materials by PIM/MIM
- Screening tests of the armour prototype materials by available high heat flux tests (thermal shock & fatigue, H/He beam load)
- Self-passivating alloys: production of larger amounts and characterization by intensive material tests

Tasks of interest:

- Characterization of self-passivating W alloys and tungsten composite materials:
  - Joint work with producers for the characterization of self-passivating alloys and W composite materials, in particular by means of Flat-top cylinder Indenter for MEchanical Characterization (FIMEC), X-ray diffraction (XRD), also at high temperature, Mechanical Spectroscopy.
- HHF tests of armour prototype materials with H/He beams in GLADIS:
  - pre-characterisation of the near surface structure
  - screening tests and cyclic loading in the GLADIS high heat flux facility
  - Post-characterisation comprising SEM and FIB analysis
- Self-passivating alloys: production of larger amounts and characterization by intensive material tests:
  - Production of larger amounts of new W alloys.
  - Identification of applicable process routes for technical scale fabrication.
  - Determination of the H & He retention and erosion of bulk material.
  - Fabrication of mock-ups and heat flux tests (GLADIS).
- Understanding of the intrinsic brittleness of W and W-alloys by investigating the dislocation movement:
  - Basic characterization of the defects and dislocation movement on a selection of standard deformed W and W alloys
  - Mechanical properties (tensile) and thermal shock resistance will be investigated with internal friction. Grades include the reference double forged pure W, single forged pure W, UHP-W, W-1%Ta, W-5%Ta, K-doped W and a W-Rhenium alloy
- Development and characterization of W-TiC alloys by pulsed electric current sintering:
  - Fabrication of material: verification of the effect of the TiC addition
  - Specific qualification and characterization: high temperature mechanical tests and e-beam heat loading
- Mutual effects of particle fluxes and transient heat loads on tungsten as a PFM. Comparison of the simultaneous loaded samples and induced surface damages with those damages induced by pure thermal or plasma exposure (JUDITH):

  - Successive exposure of tungsten to steady state heat loads/particle fluxes and transient heat loads and vice versa (variation of particle flux, fluence, particle energy, surface/base temperature, absorbed power densities)
  - Characterisation of induced thermal shock damages before and after plasma exposure, investigation of differences to pure thermal loading, dependence on plasma and e-beam parameters
  - Characterisation of induced damages/material modifications by particle fluxes before and after e-beam exposure, investigation of differences to pure particle exposure, dependence on plasma and e-beam parameters
- Manufacturing and optimization of self-passivating bulk W-alloys:
  - Mechanical characterization as a function of temperature at (3PBT, tensile) on samples with optimum microstructure and low O level of <u>WCr10Si10</u> material
  - Production of larger samples and quantities of <u>WCr12Ti2.5</u> material for different characterizations. Fabrication of mock-ups and heat flux tests (GLADIS).
  - Optimize fabrication route of alloys with higher Cr content (WCr**18**Ti2.5) and study new possible compositions.
  - Explore ways to improve the mechanical behaviour of the WCr12Ti2.5 system.
- Mechanical Characterization of novel W-based armour alloys:
  - Performance of suitable tests (for example 3-point-bending or tensile tests) to determine general material properties (strength, toughness, DBTT etc.) in dependence of temperature (T < 1600°C)
- Fabrication and optimization of different W armour materials by PIM:
  - Development of PIM materials with different chemical compositions
  - Production/fabrication of prototype grades via PIM
  - Adaptation of the heat-treatment process
  - Characterization of mechanical and physical properties
  - High heat flux testing
  - Characterization after HHF testing

WP13-MAT-HHFM-02

Structural materials for Low Temperature Cooling Concepts

This activity is dedicated to the study of Copper materials, and Low Activation Austenitic Stainless Steels. For Copper materials, ODS copper and copper composites will be considered. The main lines for the development of low-activation Austenitic SS cover standard alloys, stabilized alloys and possible new developments.

<u>Copper materials</u>

- Fabrication of copper alloys by two different routes: (1) ODS copper (e.g. Cu-Y_2O_3), and (2) copper composites (e.g. particle, wire, mesh, or foil reinforcement)

- Qualification of CuCrZr alloys to identify the optimum operation Temperature range
- Production of Cu-W gradient material (suitable for transition from CuCrZr to the W- armor)

Main objectives include:

- Development of Cu composite materials (fibre and foil reinforced copper pipes, W-Cu graded materials and Cu-(W)-laminates

Tasks of interest:

- Graded interlayer of W/Cu composites. Thermo-mechanical evaluation of infiltrated W/Cu1CrZr composites with uniform compositions :
  - Evaluation of experimentally measured tensile deformation behavior and rupture
  - Analysis of microstructural failure feature
  - Interpretation of the observed tensile behavior by means of microstructure-based finite element analysis
- Development of Cu-TaC composites:
  - Production of Cu-5%TaC composites by ball milling
  - Consolidation of the Cu-TaC composites by spark plasma sintering
  - Annealing treatments
  - Plasma exposure
  - Microstructural characterization by electron microscopy and X-ray diffraction
  - Microhardness measurements
  - Measurement of thermal conductivity
- Development of W-Ta composites. Full densification of W-Ta composites:
  - Production of W-20%Ta composites by ball milling
  - Consolidation of the W-Ta composites by spark Plasma sintering
  - Plasma exposure a
  - Microstructural characterization by electron microscopy and X-ray diffraction
  - Microhardness measurements
  - Determination of fracture toughness
  - Characterization of fracture surfaces
  - Measurement of thermal conductivity
- Testing of different routes for W-Cu FGM:
  - Powder metallurgy - partial Cu melting limit
  - Co-deposition and heat treatment
  - New powder foil composite route
  - Investigation of the role of oxide/carbides additions

WP13-MAT-HHFM-03

Structural Materials for High Temperature Cooling Concepts

This activity is dedicated to the study of long – term structural materials. Mainly to the development of W sheet materials (thin plates), and W and SiC- based composites, together with specific high temperature characterisation of this materials, i.e., Charpy, 3PB, tensiles tests, Fracture toughness, grain growth, recrystallization, creep and fatigue experiments. High performance steels production will be explored.

- Intrinsic brittleness of W and further embrittlement due to irradiation: improvement of ductility
- Development of composites (short Ta fibre, W fibre reinforcement, and W-Cu laminates)
- Characterization experiments to fill the database. Missing data for the structural tungsten materials: long-term recrystallization/grain growth, long-term creep, and low cycle fatigue

High performance steels

"Generation Four Ferritic – Martensitic steels" development, with improved high temperature creep strength (up to 650°C) achieved using Thermo – mechanical Treatment (TMT) to improve the microstructure and density of radiation defect recombination centres.

- Production of precipitation hardened EUROFER (GEN4 EUROFER)

Main objectives include:

- Fabrication and characterisation of tungsten composite materials with respect to application limits.
- Extension of the database: fracture-toughness and long term grain stability of thin W- plates.

Tasks of interest:

- Production of larger material specimens of Wf/W composites with improved properties:
  - Development and realization of new CVD production technique (layered CVD-matrix deposition)
  - Implementation of an engineered interface by magnetron sputtering in multi-fiber composites
  - Bending tests of recrystallized Wf/W-samples
  - Mechanical and structural characterization of pure CVD-tungsten (influence of annealing)
  - Assessment of NS-W fibres (stability against recrystallization
- Development W-containing composites. Incorporation of W into SiC-based composite:
  - Feasibility study of W-containing matrix in SiC-based composites and potential improvement with fibres

  - Improvement of mechanical properties of composites by improvement of interphase layer (thickness, composition)
  - Characterisation of these composites (microstructure, mechanical properties, thermal conductivity)
- Development of Cu coating technology for W laminate:
  - Optimization of Cu deposition on W foils and assembling of W-Cu stacks from coated foils
- Characterization of tungsten and tungsten alloys up to 1000°C by the indentation technique:
  - Examination with a large series of experiments of the testing capability of a cubic boron nitride indenter tip suitable for high temperature testing on hard materials
  - Tests on unirradiated tungsten samples at high temperature
  - Assessment of corresponding mechanical properties and comparison with measured properties at room temperature
- Ultramicroscopy and nano-scale composition analysis of pure-W, W-alloys and W-based composites and of final parts made by PIM:
  - Ultramicroscopy investigation of the Ta(fibre)/W matrix interface in W-Ta short fibre interface (lattice images, diffusion profiles)
  - Similar investigation of the Ta(fibre)/W matrix interface in oxide doped material (aiming at slowing the interdiffusion process)
  - Joints examination by X-EDS (with HRTEM and FIB instruments) in mock-ups
  - Ultramicroscopy and micro-composition investigation by FIB-SEM of (1) pure W made by PIM as a reference material, (2) ODS W-alloy with 1vol%Y2O3
  - Ultramicroscopy investigation of the interface of W-matrix grains with Yttria grains (evidenced the existence of that kind of grains which can influence the thermal and, perhaps, the mechanical properties of W+1vol%Y2O3 ODS alloy)
  - Ultramicroscopy investigation of alloys of composition WCr10Si10 and WCr12Ti2.5 (in wt.%) with an extremely fine microstructure (grain size below 500 nm), in order to understand the intergranular fracture behavior at 1.000 deg.C by evidencing, perhaps, the presence of impurities at the grain boundaries
- Fabrication and characterization of tungsten composite materials (laminates) with respect to application limits:
  - P.I.E. of W-Cu laminate specimens
  - Fabrication of W-X laminates where X stands for elements with high melting points and good interface compatibility with W
  - Verification of possible increase of the operation temperature by use of WVM foils
  - Development of alternative pipe fabrication routes/processes
  - Basic characterization of promising materials
  - High temperature pipe burst tests
- Production of precipitation hardened EUROFER (GEN4 EUROFER)

- Literature study
- Assessment and comparison of various precipitation elements and mechanisms
- Production and characterization of a first laboratory scale batch

- Fracture-Mechanical (FM) and microstructural characterization of tungsten alloys:

  - Investigation of the influence of the fabrication route specific anisotropic microstructure on the fracture behaviour of tungsten alloys
  - Investigation of the influence of the load rate on the fracture toughness and DBTT of tungsten alloys
  - Investigation of upper shelf fracture toughness of tungsten alloys by using J-Integral and/or Crack Opening Displacement (COD) methods
  - Performance of accompanying fractographic and microstructural investigations

WP13-MAT-HHFM-04

Material Technologies

This activity is dedicated to the study of material Technologies: Joining, and fabrication by microstructural shaping. Joining studies cover brazing W-W (structural and functional), brazing W-steel (structural joint), plasma pulse welding and possible alternatives. Fabrication by structural shaping is mainly devoted to deep drawing W, bending W and pressure forging W. Other more innovative technologies as two – or multiphase PIM/MIM, and electro – chemical layer deposit are also included in this activity.

Joining

- Structural joints for W-steel and W-W
- Functional joints for attaching the W armour to the W structure
- Brazing (Cu, Pd, Ti being used as brazing materials), and pulse plasma brazing

Fabrication by shaping the microstructure

- Development of bending, deep drawing, pressure forging or similar techniques for machining of tungsten plate materials. To be applied to mock-up fabrication.

Process development

- Development of PIM as a tool for mass fabrication of tungsten armour parts

<u>Main objectives</u> include:

- Development of fabrication processes for structural joints (W-EUROFER and tungsten-tungsten) is very important Therefore, brazing with the systems Cu, Pd, Ti and pulsed plasma welding/brazing are of highest interest.
- Investigation of multi-phase PIM/MIM to extend the fabrication process for more complex functional high heat flux parts.

<u>Tasks of interest:</u>

- Neutron diffraction qualification of interfaces in W-laminates for structural divertor applications:
  - Selection of prototype W-foil laminate and un-strained reference material
  - Neutron diffraction measurements, to be carried out at the High Flux Reactor of ILL-Grenoble
  - Data analysis, consisting in Rieteveld refinement and profile analysis of diffraction patterns as well as strain evaluation
- Development of brazing processes for W-EUROFER structural joints:
  - To set the optimum composition of Cu-Ti alloy that ensure brazing conditions and service behaviour of the W-EUROFER joint for He cooled divertor
  - Mechanical tests of the joints to assess the quality/improvement of the joint and to evaluate possible applications
- Optimisation of SITE process and joining. Study of W-coating on SiC-based composites:
  - Further increase in thermal conductivity by optimisation of the SITE process
  - Joining of structural materials
  - Characterisation of mechanical and thermal properties and gas permeability
- Electrochemical coating for joining and of mechanical joint characterization:
  - Study of material technology joining by applying electroplating for deposition of reactive interlayers and filler components to achieve good wetting and bonding of parts for. W-W, W-Eurofer, W-SS, and steel-steel.
  - Qualification of the processed joints. W-SS or W-steel joining tests by Cu-alloy will contribute to cooling modifications evaluated under actual design considerations also towards low temperature concepts.
- W+W based FGM components:
  - optimize plasma sintering process to create such components (composition, sintering parameters, shapes)
  - further development of direct pulse joining for W thin foils - steel plates
- Direct SPS joining & brazing of W to W and W to steel:
  - Production of different brazing alloys using melt spinning equipment (based on Fe, Pd, V, Cu)

  - Joining W to W and to steel by SPS using such alloys (powders and foils) and compare the results with other methods.
  - Further development of the joint quality assessment using thermal diffusion measurements in conjunction with microscopy (SEM, TEM)
- Production of real-size parts consisting of different W materials using PIM as an alternative joining process:
  - Engineering and design of a new multiphase PIM tool
  - Production of parts with the new tool
  - Adaption of the heat-treatment process
  - characterization of mechanical and physical properties
  - High heat flux testing
  - Characterization after HHF testing

WP13-MAT-HHFM-05

Demostrator Cooling Structures

This activity is dedicated to the development of "demostrator" cooling structures: Mockup fabrication and testing. Fabrication of pipes (Cu,W), channels (W), mockups with W monoblocks and with alternative designs (cooling plates, etc.) Tests of pressurized rupture, creep rupture and heat flux are included in this activity.

- Fabrication and testing of mock – ups using the newly developed or investigated materials, fabrication, and joining processes

Main objectives include:

- All kind of mockup fabrications that can be used in high heat flux tests or which clearly demonstrate the feasibility of fabrication processes.
- Mockup testing by (1) high heat flux tests and (2) pressure-rupture tests.

As in 2012, the 2013 programme will work without a specific test case. This should open the way for more or different joining and fabrication options.

Tasks of interest:

- Assessment of the thermo-mechanical behaviour of prototype cooling structures:
  - HHF screening tests in the GLADIS high heat flux facility of cooling structure prototypes
- Construction of hot-water cooling loop for GLADIS:
  - Design and start of construction
- Defect detection of prototype cooling structures (DEMO divertor fingers) before & after high heat flux tests with a non destructive method (infrared thermography):

  - Analyse (Finite Element modeling and non destructive examination) of DEMO fingers before high heat flux tests to detect defect or drift behavior
  - Analyse of DEMO fingers after high heat flux tests
  - Comparison between results obtained before and after heat fluxes treatment in order to detect the defects created during high heat flux tests
- Fabrication and testing of mockups for water cooled divertor concepts:
  - Systems engineering, design and analysis
  - Trials of manufacturing and joining processes
  - Fabrication of mockups for WC divertor concepts, to include a "stepped temperature" based concept
  - Thermal and mechanical testing of mock-ups
- Fabrication and characterization of mock-ups for water and helium cooled divertor concepts:
  - Simulation and design
  - Basic investigations on Cu-composite concepts
  - Fabrication of mockups for WC divertor concepts
  - Design and fabrication studies of demonstrators based on W laminate pipes

Resources

The estimated resources for 2013 for the MAT- HHFM research project are 4.0 ppy and 75 k€ under Priority Support

Activity	Tasks	PS manpower (ppy)	Expenditure (k€)
	Coordination	0.5	
Activity 1: Armour materials	Fabrication of a variety of different armour prototype materials by PIM/MIM	0.4	15
	Screening tests of the armour prototype materials by available high heat flux tests (thermal shock & fatigue, H/He beam load)	0.8	12
	Self-passivating alloys: production of larger amounts and characterization by intensive material tests	0.5	
Activity 3: Structural Materials for High Temperature Cooling Concepts	Fabrication and characterisation of tungsten composite materials with respect to application limits	0.8	15
Activity 4: Material Technologies	Development of fabrication processes for structural joints (W-EUROFER and tungsten-tungsten)	0.3	
	Investigation of multi-phase PIM/MIM to extend the fabrication process for more complex functional high heat flux parts	0.2	20
Activity 5: Prototype Cooling Structures	All kind of mockup fabrications that can be used in high heat flux tests or which clearly demonstrate the feasibility of fabrication processes	0.2	13
	Mockup testing by (1) high heat flux tests and (2) pressure-rupture tests	0.3	
Total allocated resources		**4.0**	**75**

Table 1: WP-2013: Human Resources and Expenditures proposed for Priority Support

1.4 Scientific and Technical Reports

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.

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.

Milestones and Deliverables

Milestones:

The results obtained within the Research Project High Heat Flux Materials 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 uploaded to the IDM database for acceptance and approval.

2. MAT-IREMEV:

Task Agreement WP13-MAT-IREMEV:
Integrated Radiation Effects Modelling and Experimental Validation

2.1 Introduction

At its 52th meeting in Marseille on 3-4 October 2012, the EFDA Steering Committee approved the EFDA 2013 Workprogramme. The Technical Specification given below outlines activities of the 2013 Work Package of MAT-IREMEV Research Project on Integrated Radiation Effects Modelling and Experimental Validation (IREMEV) of the Fusion Materials Topical Group, which is a part of the PPPT Work Programme for 2013. It will be implemented on the basis of provisions given in Art. 5 of EFDA Agreement.

2.2 Objectives

The overall objective of Integrated Radiation Effects Modelling and Experimental Validation (IREMEV) project is to develop scientifically sound physics-based concepts and mathematical models, and implement them as validated computational algorithms for predicting the rates of degradation of materials under fusion conditions, including fusion neutron irradiation and high temperatures, pertinent to the operating environment of a fusion power plant.

The IREMEV programme is based on the established principles of multi-scale mathematical modelling of materials, spanning a range of models describing interaction of neutrons with materials to changes of mechanical and physical properties resulting from the neutron irradiation damage effects. The models are applied to steels, iron-based alloys, and nano-structural composite materials, including ODS steels, and metal composites in general, for example tungsten-copper composites. It aims to create a quantitative framework for interpreting experimental tests, and predicting the performance of materials under the DEMO-relevant operating conditions.

The defining feature of the program is its focus on the science-based integration (as opposed to mechanistic linking) of a range of physically necessary models, as a guiding principle. The selection of models is made on the basis of expert assessment of the significance of the physical question that a particular model is able to address, and its place in the framework of an integrated model for a fusion power plant, treated as a complex multi-component engineering system subjected to fusion neutron irradiation. MAT-IREMEV project aims to develop capabilities needed to assess the structural integrity of components of a fusion power plant over their expected lifetime.

The modelling methods and the corresponding experimental database will also provide the basis for optimising the fusion materials experimental testing program, and for evaluating and extrapolating the relevant experimental data to DEMO-relevant operating conditions, for licensing purposes. The emphasis on the part played by modelling in the interpretation of experimental tests stems from the fact that the tests are expected to be conducted on small-scale specimens, where the data may not be interpretable using the existing rules. Activities related to modelling of high heat flux materials are integrated in a separate research project of the same Work Programme.

The Work Programme 2013 is focused on the recommendations given in the European Fusion Roadmap, and in the Assessment of the EU R&D Programme on DEMO Structural and High-Heat Flux Materials group. The priorities for the EU Materials Modelling programme for the Horizon 2020 timeframe should be:

- the development of multiscale models for the accumulation of radiation defects and transmutation products, including helium and hydrogen, in complex microstructures and complex alloys
- the investigation of fundamentals of radiation and helium embrittlement effects
- the development of models for high-temperature phase stability and microstructural stability of materials, and the determination of factors limiting the compatibility of materials under high-dose irradiation
- the problem of highly heterogeneous swelling, resulting from the highly spatially heterogeneous distribution of the neutron flux;
- the integration of models for microstructural evolution with neutron transport calculations, and the development of capabilities for the computer-model-based assessment of the end-of-life conditions for components of a fusion power plant.

The objectives of the 2013 MAT-IREMEV Work Programme are defined according to the recommendations given above, the Strategic Objectives for Fusion Materials Modelling and Experimental Validation (2010-2015) [1], and are the continuation of activities performed within WP-2008-2012.

2.3 Work Description and Breakdown

Structure

The programme is organized along five activities:

WP13-MAT-IREMEV-01

Phase Stability and Bonding

This activity is focused on predictive models for the generation of defects in materials, including HHF and structural materials, the high-temperature phase stability of candidate fusion alloys, and the accumulation of helium in Fe-Cr and Fe-Cr-Ni model alloys, as well as in EUROFER-type and ferritic steels. Special attention is devoted to the problem of high-temperature and radiation stability of oxide particles in ODS steels. The activity includes the investigation of helium and other noble gas defects, analysis of accumulation of these defects at dislocations and grain boundaries, trapping of helium at interfaces between the steel matrix and ODS particles, analysis of processing reaction pathways giving rise to the formation of ODS particles, and the investigation of interaction of defects with impurity atmospheres at high temperature.

The activity includes the investigation of (i) phase stability of Fe-Cr-Ni alloys and the kinetics of microstructural evolution of Fe-Cr alloys resulting from the combined effect of temperature and irradiation, (ii) analysis of energies for thermally activated migration of defects and dislocations, models for helium and other noble gas defects, and accumulation of helium at defects at dislocations and grain boundaries, including interaction of He and noble gas atoms with impurities for the development of a quantitative model for helium embrittlement, and (iii) assessment of reaction pathways resulting in dissolution and precipitation of oxide particles in ODS steels.

Main objectives:

- The development of atomistic methods for defect production in Fe, W, and Fe-alloys, including the effects of magnetism and high-temperature α-γ instabilities.
- Identification of pathways of migration of dislocations, for modelling brittle-ductile transitions.
- Investigation of helium and other noble gas defects, interaction of these defects with microstructures, as well as with solutes and impurities in alloys.
- Analysis of low- and high-temperature phase stability of the relevant alloys under irradiation.
- Generation of a database for modelling pathways of formation of ODS precipitates.

Tasks of interest:

- Ab initio model for the effect of He and noble-gas atoms on mechanical properties of Iron and Tungsten alloys:
  - Using first-principles modeling, evaluate the energy of interaction between He, other noble gas atoms, with edge dislocations and small defect clusters in Fe, W and other bcc transition metals, estimate changes in bulk modulus and elastic parameters, as well as changes in hardness,
  - Explore the effect of trapping of He and other noble-gas defects in nano-structures, for example interfaces between ODS particles and Fe matrix.

- Energetic, magnetic and kinetic properties of radiation defects, He and H in FeCr alloys: ab initio + AKMC studies, including:
  - AKMC simulations of radiation induced segregation in FeCr alloys
  - Ab initio investigation of vacancy interaction with He and H in dilute FeCr alloys
  - Ab initio study of energetic of vacancies, He and H at low index Fe/Cr interfaces

- Ab initio investigation of dislocations in Fe, W and other bcc metals. Identification of pathways of migration of dislocations in Fe and W as function of crystal orientation wrt to applied stress:
  - Density functional theory (DFT) calculation of the Peierls stress for ½<111> screw dislocations in iron and tungsten for various crystal orientations (-30° to +30°) using the PWSCF code and 135 atom cells containing a dislocation dipole, to assess deviations from Schmid's law in relation to the topology of the two-dimensional Peierls potential.

- Development of a validated model for the generation of primary damage in W in high-energy cascades, including the assessment of the effect of electronic stopping on the later stages of cascades generated by primary recoil atoms:
  - Simulations of high energy collision cascades in W, including the assessment of the effect of energy loss processes on the final damage configurations

- Development of cohesive models for atomistic modeling of plastic deformation, including:
  - Benchmarking of the recently developed cohesive models for Fe to select a model for the construction of Fe-Cr-based cohesive models for MD simulations
- Interaction of hydrogen with beryllium surfaces:
  - Determination of hydrogen adsorption/desorption barriers as a function of hydrogen surface coverage
  - Determination of hydrogen surface and subsurface adsorption sites and migration barriers between them
- Dynamics of defect production in iron:
  - Investigation of the evolution and production of defects in collision cascades, including the treatment of dissipative relaxation of electronic, magnetic and atomic subsystems. Development of a simulation method for the treatment of energy transfer between the three subsystems, to account for the strongly non-equilibrium nature of cascade events.
- Influence of lattice defects and elastic strain on the phase diagram and magnetic properties of candidate alloys for fusion applications:
  - Parameterize an MCE Hamiltonian, determine strain dependence of parameters of the model;
  - Perform simulations to explore the strain dependence of the Curie temperature in Fe and Fe-Cr;
  - Develop a model to enable treating atomic vibrations and magnetic excitations in alloys;
  - Parameterize interatomic interaction in the vicinity of vacancy and vacancy clusters, and apply to MC simulation of alloy decomposition at ambient and elevated temperature conditions.

WP13-MAT-IREMEV-02

Evolution of microstructure

This activity is focused on the stability and evolution of microstructure under fusion irradiation and high temperature operating conditions, integration of neutron activation and transport calculations with models for radiation defects and helium embrittlement, models for helium microstructure, assessment of sensitivity of microstructure to both the initial and environmental conditions, hardening and radiation embrittlement effects associated with the evolution of defect and dislocation networks under irradiation and thermal recovery.

<u>Main objectives:</u>

- The development of models for the evolution of helium microstructure, combining DFT, empirical potentials and AKMC models for the accumulation of helium at grain boundaries, dislocations, and impurities.
- Development of kinetic Monte Carlo models for the dissolution and re-precipitation of ODS particles, and for the assessment of the radiation stability of ODS steels.

<u>Tasks of interest:</u>

- Segregation of He and Cr at grain boundaries in FeCr alloys from ab initio and empirical-potential studies:
  - validation of empirical potentials for the description of optimized GB structures (using grand-canonical simulations way) against *ab initio* results.
  - study of the energetics and structures of small He clusters at GBs by both *ab initio* and empirical potential calculations
  - investigation of the conditions for SIA and SIA loop punching in reactions (Hen-1 + He => HenV + SIA) in the vicinity of a GB
  - Determine the lowest energy shapes of large He clusters using validated empirical potentials
- Understanding effect of carbide precipitates on dislocation mobility in steels:
  - Simulate the effect of metal carbide precipitates on the mobility of edge and screw dislocations, with the aim to provide insight and parameters suitable for the use in discrete dislocation dynamics (DDD) simulations.
- Development of structure-free AKMC to model accumulation of He on imperfections and interfaces:
  - Develop atomic-structure structure-free AKMC tool to model migration of He, formation and growth of He-bubbles at grain boundaries in pure Fe.
- Generation of a database for modelling pathways of formation of ODS precipitates. Development of kinetic Monte Carlo models for dissolution and re-precipitation of ODS particles, and for assessing the radiation stability of ODS steels:
  - Finite-temperature *ab initio* calculation of nY/n*V* complexes formed in γ-Fe at high temperature above the α-γ transition.
  - Introduction into the kinetic Monte Carlo code new energetic parameters and mechanisms, obtained from finite temperature *ab initio* calculations for γ-Fe.
  - *Ab initio* modelling of interaction between Y atoms, including Studying of Y/n*V*-complex mobility in α-Fe and investigation of factors affecting the stability of Y-O particles in α-Fe.
- Multi-scale modeling of ODS steels for fusion reactor conditions:
  - Investigate, using *ab initio* methods, the threshold for particles to break lattice symmetry
  - Develop kinetic Monte-Carlo model for simulations of ODS steels (based on Fe-Cr alloy matrix) under irradiation, to investigate effects of irradiation on ODS particle stability and evolution
- Irradiation of thin films of Fe and FeCr alloys with ions and nucleation of He-V clusters at grain boundaries in Fe:
  - Database of cascade damage in thin films of Fe and FeCr alloys
  - Development of a model for He-V cluster nucleation at two different grain boundaries in Fe as a function of temperature and He-to-vacancy ratio.
- Energy spectra of primary-recoil-atoms and secondary-energetic-particles produced in irradiated fusion materials.

- Conversion of the available database of neutron irradiation spectra into primary-recoil and secondary-energetic-particle spectra for a broad range of fusion materials

- Interaction of He with visible and invisible dislocation microstructure:

  - Using semi-empirical potentials and MD simulations, assess the strength of interaction between interstitial He and He-clusters with interstitial and vacancy dislocation loops of ½<111> and <100> types, as well as with screw and edge dislocations.
  - Study the effect of drag of He atoms decorating the loops using dislocation-loop drag model, to explore the formation, stability and evolution of He-related microstructure under fusion irradiation operating conditions

- Rate Theory modelling of He and microstructure evolution in Fe, including the simultaneous evolution of microstructure and its interaction with He:

  - Develop a Rate Theory model taking into account the evolution of dislocation loops (DL), and agglomeration of He with V generated by irradiation.
  - Develop a RT model including interaction between He and dislocation loops using binding energies derived from Molecular Dynamic and *ab initio* calculations, described in a separate task,
  - Study influence of interaction He-Dislocation Loops on the helium desorption spectra,
  - Compare/validate the model against experimental TDS spectra.

WP13-MAT-IREMEV-03

Deformation and plasticity

This activity is focused on the quantification of radiation effects on mechanical properties of materials, and includes the development of computationally efficient models for high-temperature deformation and fracture, dynamics of radiation hardening and embrittlement, α′ precipitation; sigma-, Laves-, and other phase decomposition-related embrittlement, brittle fracture of ODS steels, the synergetic hydrogen and helium effects, temperature-dependent dimensional changes in alloys induced by irradiation and transmutation.

<u>Main objectives</u>

- Analysis of interaction of dislocations with precipitates and phase inclusions, to rationalize the observed embrittlement of irradiated materials.
- Assessment of synergetic effect of combined accumulation of hydrogen and helium on microstructure, including swelling and embrittlement.
- Development of computationally efficient models for ensembles of interacting dislocation and defect microstructures, and radiation hardening of materials.
- Assessment of hardening impurity effect in the low and high temperature limit, including the dislocation dynamics based model for the synergetic effect of radiation damage and impurity atmospheres.

<u>Tasks of interest:</u>

- Assessment of hardening due to voids, dislocation loops and He-bubbles:

- Develop a DD tool to model interaction between ensembles of dislocations with radiation defects including He (voids, bubbles and dislocation loops) in pure Fe

- Interaction of dislocations with phase inclusions:
  - Assess the strength of interaction between M6C and M23C6 Carbides and σ-phase Cr precipitates
  - Develop a database for the implementation of interaction mechanisms and related obstacle strengths in dislocation dynamics methods

- Molecular Dynamics study of the energetic properties of H-He-V bubbles in Fe, in order to predict the simultaneous evolution of H and He in Fe, and their possible synergistic effects, the energetic properties of the clusters/bubbles they form by agglomeration must be determined:
  - Implement a range of semi-empirical potentials for the interactions H-H, He-He, Fe-Fe, H-Fe, H-He, He-Fe,
  - Calculate the formation/binding energies of large H-He-V bubbles as a function of the H/He and He/V ratios,
  - Investigate the influence of H on the binding energies of He and V to bubbles,
  - Transfer results as input for kinetic model to be developed in a separate task to investigate synergistic effects between H and He.

- Rate Theory modelling of synergistic evolution of H and He in Fe. Growth of H-He-V bubbles:
  - Use energetic properties of H-He-V bubbles derived from Molecular Dynamics calculations (described in a separate task),
  - Investigate eventual synergistic effects under realistic experimental conditions: fusion and triple beam irradiation,
  - Investigate the effect of H on swelling.

WP13-MAT-IREMEV-04

Material Science and Simulation of armor materials and joints

This activity is dedicated to the simulation and prediction of irradiation performance of armor materials and joints; understanding of basic mechanism of materials behavior, modeling of macroscopic material properties; and a part of Validation experiments (JANNuS, micromechanics, etc). Tasks will be devoted to the study of:

- Intrinsic brittleness of W and further embrittlement due to irradiation and/or transmutation. Simulation of irradiation damage as well as the validation experiments (JANNUS, etc.)
- Plasticity studies for the case of W-Re
- Micromechanical tests applied to study of either irradiated specimens or to the examination of specific grain boundaries
- Modelling of macroscopic material properties for contributing the irradiation properties database (filling in gaps by inter- and extrapolation)

Main objectives:

- Intrinsic brittleness of W and its embrittlement due to irradiation and/or transmutation effects
- Simulation of irradiation damage as well as interpretation of validation experiments (JANNUS, etc.)

Tasks of interest:

- High temperature properties of vacancy and interstitial type defects in tungsten:
  - DFT calculation of the formation entropy of mono- and di- vacancies in W
  - DFT calculation of the migration entropy of mono- and di- vacancies in W
  - DFT calculation of the formation entropy of mono- and di- interstitials in W
  - preliminary FPKMC simulation of isochronal resistivity recovery experiments in W
- Calculation of dislocation kink-pair formation enthalpy in W from first principles:
  - DFT calculation of the line tension in tungsten using the PWSCF code and 135 atom cells containing a dislocation dipole
  - Computation of the kink-pair formation enthalpy with the line tension model using the DFT inputs
- Simulation of radiation damage in tungsten with He and H production in order to predict the evolution of the microstructure and the possibility of swelling or blistering using kinetic Monte Carlo: Kinetic modeling of He (H) and dpa in tungsten
- Investigation of vacancy defects in W: interactions with He and H isotopes:
  - Model, by OKMC, helium evolution in tungsten based on previous results on He release and Positron Annihilation spectroscopy (PAS): focus on the low dpa/He ratio
  - Identify Hex-Vn complexes by comparison with DFT calculations of their positron annihilation characteristics
  - Perform an experimental study on W/He/H accumulation in Jannus for the dpa/He ratio lose to the one expected in DEMO: probing of the region where He is implanted by using PAS and TEM to study temperature and damage dose effect on vacancy defects formation.
  - H dedicated experiments to validate OKMC parametrization for Hydrogen in tungsten
- Understanding deformation and fracture behavior of W-Re alloys and specimens containing grain boundaries on the micrometer scale:
  - Production of micrometer-sized samples using the ion slicing method. Material: recrystallized and recovered tungsten and a tungsten-rhenium alloy (W-26wt%Re)
  - in-situ testing of the specimens. Two populations of specimens: notched and unnotched
  - evaluation of material parameters such as strength and especially grain boundary fracture toughness
- Creation, clustering and mobility of hydrogen isotope trapping defects in tungsten:
  - Identify the mechanisms how vacancy type defects are created in W at H supersaturation conditions with MD

- Check if vacancy type defects are created in W at H irradiation energies below the displacement threshold energy with MD
- Check what type of self-interstitial atom (SIA) clusters form in W with MD
- Calculate binding energies of SIA clusters in W with MD and DFT

- Evolution of dislocation loops and their contribution to hardening in W:

  - Understand the formation mechanism of, the interaction between and mobility of dislocation loops in BCC W.
  - Perform medium term annealing of cascades at the µ-seconds time scale i.e. well beyond MD simulations.

WP13-MAT-IREMEV-05

Experimental validation of models

This activity is dedicated to the experimental validation of models. In the ion-irradiation experiments the specific questions include the analysis of dose rate effects, defect accumulation and patterning, defect and dislocation microstructures, micromechanical tests. Helium accumulation and micro-fracture, Helium – Hydrogen synergetic effects, grain boundary and surface effects, and dimensional changes associated with the accumulation of radiation damage. The advanced characterization methods involve applying both *in–situ* and *ex-situ* electron microscopy, advanced TEM, micromechanical tests, SANS, PAS, EELS, and APT.

Main objectives:

- Exploration of the effect of chemical composition, specifically Cr content, on the swelling of ion irradiated FeCr alloys.
- Exploration of He – H synergetic effects on Fe, FeCr alloys and steels.
- Experimental and modelling investigation of thermal desorption of helium from ferritic materials and refractory alloys.
- Quantitative analysis of neutron irradiation induced microstructural defects in reduced activation ferritic/martensitic steels from ARBOR and SPICE irradiations. SANS investigation.
- Assessment of phase stability and defect microstructure in Fe-based alloys, steels and ODS materials under high-temperature irradiation.
- Experimental investigation, linked with dislocation dynamics modelling, of the effect of impurity atmospheres on hardening, softening and embrittlement of materials the low- and high-temperature limits.
- Experimental and modelling analysis of in-situ electron microscope observations of defect accumulation and microstructural development in Fe-based alloys and steels.

Tasks of interest:

- Effect of Cr and of the reinforcement nanoparticles on the swelling of ion irradiated FeCr and ODS alloys:

  - In-situ and ex-situ ion irradiation of model FeCr alloys in mono-beam and dual-beam modes at Jannus
  - TEM characterization of the dislocation microstructure and the void swelling of the model FeCr alloys after radiation exposure

- Helium behavior in Fe-based materials studied by coupling TDS, TEM and SIMS:
  - Characterization of Fe-Cr samples, implanted with He within the WP12 task, by coupling a set of techniques:
    - Thermal helium Desorption Spectroscopy (TDS) characterization of He implanted Fe-Cr alloys for two implantation energies (8 and 60 keV) and two fluences (1014 and 1016 He/cm2); comparison with results obtained in the WP12 task on pure Fe samples.
    - Transmission Electron Microscopy (TEM) characterization after implantation as well as after heat-treatment. For middle energy implantation (60 keV), cross section observations are foreseen to better characterize He species (bubbles) evolution.
    - SIMS characterization of 60 keV implanted materials after implantation and after heat treatment to depth profile He in both Fe-Cr systems and compare the effect of Cr concentration in He diffusion process.
- Open Access to JANNUS: Simulation and prediction of irradiation performance of Fe-Cr model alloys, steels, armor materials and joints; Validation experiments using the JANNUS irradiation platform
- Formation of vacancy defects and their interaction with impurities in irradiated Fe and Fe-Cr alloys:
  - Y, Ti and O implantations in pure Fe and FeCr. Positron annihilation Spectroscopy (PAS) and SIMS to follow the nature of vacancy defects, the formation of vacancy defects- impurity complexes and the impurity depth profiles in as-implanted and in post annealing samples. Comparison with theoretical data (DFT): V-Imp dissociation.
  - PAS measurements in low energy implanted Fe samples in combination with complementary analysis such as TEM,TDS to better understand the role of He in the swelling.

- Quantitative analysis by SANS investigation of neutron irradiation induced defects in reduced activation ferritic/martensitic steels from ARBOR and SPICE (B-alloyed Eurofer97) irradiations:
  - Selection of the SPICE and ARBOR samples to be investigated by SANS (both kinds neutron irradiated with 16 dpa, at 250°C and 450°C, for SPICE with B concentrations corresponding to helium content of 5000 appm)
  - SANS data analysis , determination of size distributions for helium bubbles (SPICE) and other microstructural radiation defects (ARBOR), comparison with information available by TEM to provide a reliable experimental determination of metallurgical parameters necessary for validation of theoretical models
- Evaluation of He effects on Eurofer and EU-ODS Eurofer by nano-indentation and TEM:

- He implantation with box-profile configuration between 2-15 MeV with fluence of 1.67. 1015 He ions/cm2. The implantation will be performed at room and elevated temperatures.
- Nano-indenation tests.
- Nano-griding tests.
- Detailed microstructural investigations by FIB and TEM in different zones of the damage layer in order to compare the microstructural changes produced in function of the He concentration.

- Microstructural characterization of irradiation induced effects:
  - Specimens preparation
  - TEM characterization of prepared specimens
  - Evaluation of statistical data, TEM images

- Quantitative TEM investigation of neutron irradiated induced defects in RAFM steels from ARBOR and SPICE irradiations**:**
  - STEM-EDX investigation of grain boundary segregation in 15 & 32 dpa @330 °C irradiated EUROFER97 (WTZ, ARBOR1)
  - TEM-EFTEM analysis to look for α‘ precipitation in 15 & 32 dpa @330 °C irradiated EUROFER97 (WTZ, ARBOR1)
  - Quantitative TEM analysis of selected EUROFER97 specimens irradiated to 15 dpa@300°C (SPICE) to study the influence of neutron flux
  - Quantitative TEM Investigation of 70 dpa irradiated EUROFER97 and boron containing steels depending on availability of ARBOR2 specimens

- Characterization of RAFM steels up to 650°C by the indentation technique:
  - Identification of indentation-derived mechanical properties of RAFM steels for different testing temperatures

- Short-range order kinetics in Fe-Cr alloys under irradiation by electrical resistivity measurements:
  - Higher temperature measurements (up to T=700 K) to obtain information on ordering vs. T and concentration
  - Variation of the defect generation rate (irrad. flux) – to obtain information on sink strength
  - Distinction between vacancies/interstitials
  - Finding correlation between resistivity and SRO by combining resistivity and Mössbauer measurements in Fe-5Cr
  - Detailed modeling integrating all effects (irradiation, migration, ordering)
- Resistivity Recovery of proton irradiated Fe-Cr alloys at different dose levels:
  - Resistivity recovery studies at different dose levels (low-medium-high dose) on 10 and 15 %Cr concentrations samples

- Iron ion irradiation effects on the magnetic and structural properties of Fe thin films:
  - Irradiations at JANNuS facility at low doses and different dose rates
  - Polarised neutron reflectivity measurements on irradiated samples
  - Analysis of the data
  - Mössbauer measurements

Resources

The estimated resources for 2013 for the MAT- IREMEV research project are 7.50ppy and 110 k€ under Priority Support

Activity	Tasks	PS manpower (ppy)	Expenditure (k€)
	Coordination	0.5	
Activity 1: Phase Stability and Bonding	The development of atomistic methods for defect production in tungsten, Fe and Fe-alloys, including magnetism and high-temperature α-γ instabilities	1.3	
	Identification of pathways of migration of dislocations, for modelling brittle-ductile transitions	0.7	
	Investigation of helium and other noble gas defects, interaction of these defects with microstructures, as well as with solutes and impurities in alloys.	0.3	
	Generation of a database for modelling pathways of formation of ODS precipitates.	0.2	
Activity 2: Evolution of the microstructure	The development of models for evolution of helium microstructure, combined DFT, empirical potentials and AKMC models for the accumulation of helium at grain boundaries, dislocations, and at impurities.	0.6	
	Development of kinetic Monte Carlo models for dissolution and re-precipitation of ODS particles, and for assessing the radiation stability of ODS steels.	0.2	

	Study of Energy spectra of primary-recoil-atoms and secondary-energetic-particles produced in irradiated fusion materials.	0.5	
Activity 3: Deformation and plasticity	Analysis of interaction of dislocations with precipitates and phase inclusions, to rationalize the observed embrittlement of irradiated materials.	0.5	
	Assessment of synergetic effects due to accumulation of hydrogen and helium on microstructure, including swelling and embrittlement.	0.3	
	Development of computationally efficient models for ensembles of interacting dislocation and defect microstructures, especially in the high temperature limit.	0.4	
Activity 4: Material Science and Simulation in armor materials and joints	Simulation of irradiation damage as well as the validation experiments	0.2	10
Activity 5: Experimental validation of models	Exploration of the effect of chemical composition, specifically Cr content, on the swelling of ion irradiated FeCr alloys.	0.3	
	Exploration of He – H synergetic effects on Fe, FeCr alloys and steels.	0.5	20
	Quantitative analysis of neutron irradiation induced microstructural defects in reduced activation ferritic/martensitic steels from ARBOR and SPICE irradiations. SANS investigation	0.8	
	Experimental and modelling analysis of in-situ electron microscope observations of defect accumulation and microstructural development in Fe-based alloys and steels.	0.2	80
Total allocated resources		**7.5**	**110**

Table 1: WP-2013: Human Resources and Expenditures proposed for Priority Support

2.4 Scientific and Technical Reports

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.

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.

Milestones and Deliverables

Milestones:

The results obtained within the Integrated 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 uploaded to the IDM database for acceptance and approval.

References

[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

3. MAT-ODSFS:

Task Agreement WP13-MAT-ODSFS:
Nano-structured ODS Ferritic Steel Development

3.1 Introduction

At its 52th meeting in Marseille on 3-4 October 2012, the EFDA Steering Committee approved the EFDA 2013 Workprogramme. This Technical Specifications corresponds to the activities of the 2013-WP of MAT-ODSFS Research Project on Nano-structured ODS Ferritic Steel Development (ODSFS) of the Fusion Materials Topical Group in the PPPT WP 2013. It will be implemented on the basis of the provisions given in Art. 5 of EFDA Agreement.

3.2 Objectives

The objective of the present programme is to develop ODS ferritic steels with high tensile and creep strength and sufficient ductility and fracture toughness up to about 750°C, as well as good radiation resistance. The strategy for achieving this objective consists in optimizing the chemical composition and manufacturing conditions at the laboratory scale and, at the same time, launching the fabrication of ODS ferritic steels at semi-industrial or industrial scale.

The Work Programme 2013 is focused on the recommendations given in the European Fusion Roadmap, and in the Assessment of the EU R&D Programme on DEMO Structural and High-Heat Flux Materials group, addressing the following issues:

- Low ductility and fracture toughness at room temperature of current ODS High Cr
- Low fracture toughness for non uni-directional/complex shape applications
- Lack of industrial-scale fabrication technology. Reproducibility
- Lack of comprehensive materials property data
- Helium transmutation embrittlement/hardening/dimensional stability/ under irradiation

3.3 Work Description and Breakdown

Structure

The programme is organized along four activities:

WP13-MAT-ODSFS-01

Production and characterization of laboratory-scale batches of nano-structured ODSFS

This activity is devoted to optimizing the chemical composition and manufacturing conditions involving powder metallurgy. Chemical composition should be (13-14)Cr-(1-2)W-0.3Ti+0.3Y2O3. Mechanical alloying, followed by either hot isostatic pressing (HIPping) or hot extrusion and thermo-mechanical treatments, like cross hot rolling, high speed hot extrusion, etc., will be used to obtain a dense population of small nano-clusters and submicrometre grains, required for high creep strength and reasonable fracture toughness after irradiation. Small batches up to about 1 kg will be produced at the laboratory scale.

Characterization before irradiation of the produced ODSFS will be done. This includes microstructural investigation and mechanical characterization:

- Microstructural investigation: Optical microscopy, SEM, TEM, APT, SANS, XRD, laser confocal microscopy, chemical analyses, etc.
- Mechanical characterization: Tensile tests, compression tests, fatigue tests, Charpy impact tests, fracture toughness measurements, microhardness measurements, nano-indentation experiments, etc.

A selection of the most promising produced materials will be done, to start a characterization programme to correlate changes in the mechanical and physical properties with changes in the microstructure. A data base of all these properties for the produced materials should be done for comparison of results.

The main objectives of this activity are:

- To produce a material with higher ductility and fracture toughness at room temperature, with sufficient fracture toughness.
- To create a comprehensive materials property data of non - irradiated material.

<u>Tasks of interest:</u>

- Production and characterization of ODS FS at laboratory scale in a reproducible process:
  - Production and characterization of laboratory scale batches of nano-structured ODSFS starting from a fixed composition and subsequent characterization (data base of non – irradiated material). Mechanical alloying, followed by hot isostatic pressing (HIP) will be used to obtain the sample to be characterized. Small batches up to about 1 kg will be produced at the laboratory scale.
- ODSFS by improvement of precursor and Spark Plasma Sintering processing. Powders/ribbons will be prepared by splat quenching and planetary milling:
  - Powders/ribbons will be investigated by structural, microstructural measurements and Mossbauer spectroscopy
  - As prepared powders will be subject to SPS. SPS with different heating rates for microstructure control trying also to adjust the specific features of powders with SPS conditions.

  - Samples will be characterized by XRD, SEM/EDS, Vickers hardness/toughness. Selected samples will be investigated by Charpy/tensile/compression/and magnetic measurements.
  - Reproducibility aspects and different initial compositions will be approached pending on progress.
- Optimization of the chemical composition and manufacturing conditions at the laboratory scale of ODS ferritic steels:
  - Study of the influence of the process control agent, PCA, (in correlation with other milling parameters) on the mechanical properties and density of ODSFS's
- Inspection of TMT routes to improve the mechanical properties of ODS steels:
  - Production of laboratory scale batches by MA+HIP
  - Microstructural and mechanical characterization of the produced alloys in as-HIP state and after TMT (forging, hot rolling or forging+hot rolling).
  - Comparison with other results following different characterization techniques: Density measurements in a He ultrapycnometer, Determination of O and C using LECO analyzers, XRD, SEM, TEM, SANS, APT, Microhardness measurements, Tensile testing, Charpy impact testing
- Production of a 5 kg batch of ODSFS:
  - Production (powder fabrication, mechanical alloying, HIP, hot-rolling) of a 5 kg batch and basic characterization (microstructure, tensile, Charpy)
- Fabrication and characterization of ODS steels by new methods, using MA powders:
  - Fabrication of ODS steel by hot pressing
  - Cold spray of ODS steel layer on Eurofer 97
  - Preparation of bulk ODS steel by cold spraying and pressing

WP13-MAT-ODSFS-02

Production and characterization of industrial batches of nano-structured ODSFS

This activity is focused on the fabrication of ODS FS using industrial scale-methods. Investigate feasibility of production of ODSFS in large batches. Chemical composition should be (13-14)Cr-(1-2)W-0.3Ti+0.3Y2O3.

Following the identification of chemical composition and manufacturing conditions, production of one or several batches and preliminary characterization of the batche(es) in the unirradiated condition have to be carried out. The characterization activities should be comparable to the ones described under the previous line, but should also include creep and ageing experiments as well as analysis of the physical properties (thermal, electrical and magnetic properties).

A selection of the most promising produced materials will be done, to start a characterization programme to correlate changes in the mechanical and physical properties with changes in the microstructure. A data base of all these properties for the produced materials should be done for comparison of results.

The main objectives of this activity are:

- Production of ODS FS at industrial scale in a reproducible process
- ODS FS tube manufacturing
- To create a comprehensive materials property data of non – irradiated material

Priority task: Industrial or semi-industrial scale fabrication of ODSFS

Tasks of interest:

- Production and characterization of ODS FS at industrial scale in a reproducible process:
  - Production and characterization of industrial batches of nano-structured ODSFS with a fixed subsequent characterization (data base of non – irradiated material) in a reproducible process.
  - tensile and charpy laboratory tests at room and high temperature
- Industrial production of nano-structured ODS FS following a simplified route (avoiding the MA step), improving reproducibility:
  - Atomization of ferritic stainless steel powder with nominal Fe-14Cr-2W-0.3Ti-0.233Y composition (including dispersoid forming elements, Ti and Y) and the required O content
  - Selection of adequate thermal treatment(s) to obtain a dense material with the desired nano-metric oxide dispersion.
- Production of a 10kg batch of ODSFS:
  - Production (powder fabrication, mechanical alloying, HIP, hot-rolling) of a 5 kg batch and basic characterization (microstructure, tensile, Charpy)

WP13-MAT-ODSFS-03

Ion Irradiation and post-irradiation characterization of produced nano-structured ODSFS

Acquire information about the irradiation-induced microstructure changes, with a focus on the stability of oxide particles, and effects of radiation hardening by performing ion irradiations of the laboratory scale batches in the JANNuS facility under various conditions as well as post-irradiation characterization.

It also includes the definition of irradiation conditions, irradiation experiments (including eventually in-situ TEM) and post-irradiation characterization of the batches. Post-irradiation examination (PIE) will include TEM analyses and hardness measurements.

A data base of all these properties for the produced materials should be done for comparison of results.

The main objectives of this activity are:

- Study of Helium transmutation embrittlement/hardening/dimensional stability (swelling)/ under irradiation
- Link the changes in the microstructure under irradiation with changes in the mechanical properties

<u>Tasks of interest:</u>

- Transmission electron microscopy and positron annihilation spectroscopy analyses of single and triple ion irradiated ODS Fe (12-14)Cr steels:
  - Post-irradiation characterization by transmission electron microscopy and positron annihilation spectroscopy of an ODS Fe-14Cr-0.3Y2O3 alloy simultaneously irradiated with Fe + He + H at 600ºC up to 30. Characterization should focus in determining the irradiation induced microstructural evolution of these alloys (microstructural changes, development of dislocation loops, irradiation induced segregation, stability of the secondary phases present in the alloys).
  - Simultaneous triple ion implantation (JANNUS) of an ODS Fe-14Cr-0.3Y2O3 alloy under similar conditions as the ones to compare the microstructures
- Evolution of the nano-structures of ODS steels under ion irradiations characterized by Atom Probe Tomography and Electron microscopy:
  - Investigation of stability at very high dose – 250 dpa of ODS steels irradiated at 500°C
  - Study of the stability of the microstructure of ODS steels under ion irradiations at higher temperature (700°C)
  - Investigation of the microstructure by TEM and APT that will bring information about dose effect (by comparing microstructure before and inside the peak damage) and the temperature effect
- Microstructural characterization, by means of small-angle neutron scattering (SANS) and neutron diffraction, of laboratory nano-structured ODSFS submitted to HIP extrusion, rolling and other relevant thermo-mechanical treatments:
  - SANS measurements of the selected laboratory nano-structured ODSFS and data analysis providing size distributions of the nano-clusters
  - High resolution neutron diffraction measurements of the selected laboratory nano-structured ODSFS and crystallographic data analysis by Rietveld refinement
  - Correlation of the obtained results with other available metallurgical information to correlate changes in mechanical and physical properties with microstructural evolution.
- Microstructural investigations of Fe-Cr ODS alloys and 9Cr martensitic steels irradiated to high doses:
  - TEM investigations focused on the microstructure of point defect clusters (dislocation loops, cavities) after irradiation in the different alloys (determination of size distributions/number densities)
  - Preparation in hot-cell of a plate using an MA957 sample irradiated to 78 dpa to be used for subsequent SANS experiments.
  - Installation in hot-cell of a new dedicated saw and preparation of "matchstick" specimens using MA957 irradiated to 42 dpa

WP13-MAT-ODSFS-04

State of the art of nano-structured ODSFS: Literature review

This activity is devoted to the evaluation of the available information about nano-structural ODSFS produced in the USA, Japan and India.

Tasks of interest:

- Report about the state of art of Nano-structured ODS Steel Developments

Resources

The estimated resources for 2013 for the MAT- ODSFS research project are 2.0 ppy and 45 k€ under Priority Support

Activity	Tasks	PS manpower (ppy)	Expenditure (k€)
	Coordination	0.2	
Activity 1: Production and characterization of laboratory-scale batches of nano-structured ODSFS	Production of ODSFS with a fixed composition and subsequent characterization (data base of non – irradiated material)	0.6	10
Activity 2: Production and characterization of industrial batches of nano-structured ODSFS	Production of ODSFS at industrial scale with a fixed composition and subsequent characterization (data base of non – irradiated material)	1.0	30
Activity 3: Irradiation and post-irradiation characterization of produced nano-structured ODSFS	Investigation of irradiation – induced microstructure changes, focusing on the stability of oxide particles and effects of radiation hardening on the produced material (data base of irradiated material)	0.2	5
Total allocated resources		**2.0**	**45**

Table 1: WP-2013: Human Resources and Expenditures proposed for Priority Support

3.4 Scientific and Technical Reports

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.

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.

Milestones and Deliverables

Milestones:

The results obtained within the Research Project Nano-structured ODS Ferritic Steel Development 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 uploaded to the IDM database for acceptance and approval.