STRATEGIC OBJECTIVES FOR FUSION MATERIALS MODELLING AND EXPERIMENTAL VALIDATION (2010-2015).

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Executive summary

This document gives a summary of key recent results achieved by the EFDA materials modelling and experimental validation programme, and outlines specific future objectives that, if achieved, will bring the programme to the goal of having available a comprehensive yet conceptually transparent predictive model for EUROFER-type steels.

The breakdown of objectives given in the document goes beyond stating general needs, and highlights the key physical phenomena, the development of mathematical description and experimental validation for which should advance the program to a level where computer modelling becomes capable of driving innovative development of promising candidate fusion materials.

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1. Summary

This document gives projections and outlines issues that the EFDA fusion materials modelling programme is expected to address on the timescale of five to seven years, using the presently available scientific methodology and concepts, mathematical algorithms, and the existing computer facilities. In selecting the problems and in identifying suitable approaches to solving them, we focus on materials science problems foreseen in connection with DEMO technologies, and the need to select materials for the IFMIF testing programme. Some of the issues may also be relevant to ITER operation. We highlight the development needs and generic problems, resolving which requires broadening scientific expertise in the Associated Laboratories and long-term effort. We highlight the need to devote substantial resources to quantitative experimental tests linked to mathematical modelling.

2. Introduction

There are no means for obtaining reliable quantitative information about the nature of potential breakdown modes related to performance of materials in a DEMOnstration fusion power plant. Operation of the present generation of fusion devices including Tore-Supra, Asdex Upgrade, and JET has already highlighted a range of generic materials-related problems not foreseen in the past, for example the problem of materials compatibility in the divertor, or the fact that a substantial amount of tritium can be retained in the plasma-facing materials. ITER is expected to present a broader range of issues related to materials and technology, involving plasma facing and possibly structural (in particular divertor) materials.

The analysis given below, and aiming mainly at DEMO, is based on interpolations based on the recent developments in theoretical modelling, as well as on new information from nuclear reactor tests. The increasingly large amount of information is coming from simulated irradiation experiments (ion implantation, and *in-situ* electron microscope observations).

In the rapidly developing field of fusion materials modelling it is tempting to stretch a model beyond its range of validity. The conditions of validity themselves are often difficult to establish. Application of models beyond their range of validity leads to artefacts in predictions and disagreement between predictions made using alternative approaches, with confusing outcomes where *significant* features are not correctly described. Noting the limits of the currently available knowledge and capabilities, we provide a framework that ensures the expansion of quantitative knowledge and expertise required for making informed choices for IFMIF materials test matrix, and DEMO.

An experimental programme on validation and tests is an essential and crucial part of the modelling programme, and in fact *the only* part of the programme that, by comparing predictions with experimental observations, can identify and eliminate errors potentially involved in a particular model or a concept. We believe that every task on materials modelling

(listed below in the Specific Objectives section) must involve quantitative comparison with appropriate validation experiments.

The third significant aspect of a strategy is to ensure the availability of expertise, facilities, and knowledge-based management of financial and human resources. Future work will therefore have to involve critical assessment of links between the modelling programme and practical materials development, involving industrial production and processing of novel materials.

3. General Framework

There are three general points related to the choice and performance of structural and plasma facing materials that have direct implications for the selection of modelling methods:

- Materials are expected to operate in the high-temperature domain, and operation may involve numerous shutdown events, each resulting in large temperature fluctuations.
- High energy neutron irradiation and direct bombardment of surfaces by energetic ions strongly influence the phase stability of materials in comparison with phase diagrams based on conventional equilibrium thermodynamics.
- Only sufficiently complex materials solutions can accommodate non-trivial requirements. Hence, (i) *concentrated* binary or ternary alloys, forming stable phases and microstructures under irradiation within the appropriate range of operating temperatures and irradiation dose rates, or (ii) *designed pre-fabricated microstructures* exhibiting long-term stability under irradiation, are the two promising routes for the innovative development of fusion materials.

4. Chemical Composition, Microstructure, and Heterogeneous/Complex Multi-Phase Materials

There are two variable “parameters” that can be adjusted, within reason, for a macroscopically homogeneous material to fit engineering requirements. They are (i) the chemical composition of the material and (ii) its microstructure.

The choice of composition means mixing, in certain proportions, the elements of the Periodic Table, excluding those that are harmful and cannot be contained, or those producing unacceptably high levels of radioactivity due to transmutation processes caused by the fusion neutrons. For example, the selection of chemical composition of reduced-activation steels involves replacing carbide-forming niobium and molybdenum by tantalum and vanadium (chemically similar to niobium) and tungsten (chemically similar to molybdenum). Also, the residual impurity content of aluminium, cobalt, nickel and copper has to be kept as low as possible.

The microstructure of a material, i.e. the specific arrangement of atoms on the micro- and meso-scales between one and four orders of magnitude greater than the interatomic distance, determines its engineering properties. Microstructure is formed as a result of processing of the material, for example thermal or mechanical treatment. Examples of microstructural features are crystal grain structures, grain boundaries, dislocations and dislocation structures, dispersoids formed during mechanical alloying, multiphase structures self-forming during thermo-mechanical treatment. The stability of microstructures in the environment of a fusion power plant, where the combined effect of high temperatures, stresses and irradiation gradually alters the initial microstructure, is the key aspect that characterizes engineering performance in a fusion environment.

A material used in an engineering application is *macroscopically* heterogeneous. For example the microstructure of a weld, where steel was re-heated, is different from the microstructure of

a bulk material. An interface between two dissimilar materials (for example tungsten attached to steel or copper substrate) is a two-dimensional object exhibiting properties entirely different from those of materials on the either side of the interface. Finally, a *surface*, i.e. a material-vacuum or material-plasma interface, has its own properties that can only be partially related to the bulk properties of the material.

The general objective for a fusion materials modelling programme is the development of a consistent conceptual mathematical framework for rationalising the already available experimental information on existing materials and systems, and for extending the known properties/performance parameters into the range of environmental parameters (temperature, stress, engineering strain rates, long timescales, irradiation, chemical corrosion) that are either not accessible, or which have not yet been investigated by direct experimental tests.

Applying this methodology to EUROFER, and similar steels or alloys, remains the central objective of EFDA materials modelling programme. Extending and applying the methods and algorithms to other materials, for example ODS steels, tungsten, beryllium, and other potential ITER- and DEMO-relevant materials and systems, is expected to become a part of the general scope of the fusion materials modelling programme in the near future.

5. The Current Status of Activities

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The initial objective for the programme set in 2002 was to develop a conceptual framework and computational tools for modelling radiation effects in EUROFER steel under fusion-reactor-relevant conditions in the range of operating temperatures up to 550°C, high irradiation dose approaching 100 dpa, in the presence of significant amount of transmutation products, including He and H. The proposed route to achieving this general objective was to develop physically based computational tools, which were to be validated by experiments at the relevant scale using pertinent system such as dedicated model-alloys. These computer modelling tools and the associated experimental data-bases were expected to provide the fundamental basis for interpolating the data obtained with various neutron spectra in Materials Testing Reactors, Fast Neutron Reactor, Spallation sources and ion beam irradiation experiments and, in the future, in the IFMIF facility.

The progress made so far is described below for the five main areas of the modelling programme, now the MAT-REMEV Research Project: (i) Point defects and He accumulation, (ii) Phase stability and phase diagram, (iii) Tools for large scale atomic simulations, (iv) Fundamentals of mechanical deformations and microstructural evolution, and (v) Experimental Validation.

The Annex gives a list of publications supported by this 2003-2008 EFDA programme on Modelling Radiation Effects.

Point defects and He accumulation:

Density functional theory (DFT) calculations have proven to be very effective in providing accurate information on the energetics of point defects, including the formation and migration energies, for α-Fe and other body centred cubic (bcc) transition metals. Also, DFT calculations for the first time made it possible to quantitatively estimate the energies of formation and dissociation of defect complexes involving vacancies, He and C atoms in α-Fe, without the need to refer to experimental data. The ~0.1 eV accuracy of DFT calculations is

several times better than the spread of experimental values on defect formation energies, and in this respect the new calculations represent a serious step forward in the development of a quantitative treatment of radiation effects in materials. The sufficiently high accuracy of DFT calculations makes it possible to use the calculated values for parameterising various time-dependent models for microstructural evolution.

The quantitative prediction of annealing stages on the isochronal electrical resistivity recovery curves in pure α-Fe, based on Event Monte Carlo simulations and energies of point defects and small clusters calculated by DFT, resulted in the development of a comprehensive approach to the description of experimental observations, for example the number of recovery stages and their position on the temperature scale, at the ~10K accuracy level. The effect of irradiation dose was well reproduced, as well as the effects due to the presence of carbon.

Rate Theory models were developed in order to treat events that were expected to occur during He-desorption from He-pre-implanted α-Fe sample containing a limited amount of carbon in the ~50 appm range. A Rate Theory model, parameterised using DFT-calculated energies of point defects, small clusters, and their interaction with carbon and helium, reproduced very well the experimental data on kinetics of isothermal desorption of helium for a broad range of desorption temperatures over the experimentally explored time domain.

Phase stability and phase diagram

DFT calculations of the enthalpy of mixing for various Fe-Cr configurations explained the results of neutron scattering observations that suggested the high solubility of Cr in the Fe-rich domain of the phase diagram, and the tendency towards ordering in the alloy in the concentration range below 10% Cr. Also, calculations explained the tendency towards Cr clustering above the 10% concentration threshold, in agreement with neutron diffraction data. Analysis of DFT calculations showed that local order in Fe-Cr alloy and Cr solubility is controlled by magnetic interactions between Cr and Fe atoms.

The Cluster Expansion (CE) and Magnetic Cluster Expansion (MCE) approaches were developed for large scale simulations of Fe-Cr alloys to assess the phase stability of the alloys in the entire range of concentrations and temperatures. Using Exchange Monte Carlo (EMC) simulations, the CE predicted the Cr solubility limit corresponding to the experimentally observed range of occurrence of α/α' phase decomposition, confirmed by test calculations over a range of temperatures. Nevertheless, as magnetism was not explicitly treated, the predictive capabilities of the CE approach remained limited. The MCE-based approach involving both short-range direct interactions between atoms as well as contribution to the free energy resulting from fluctuations of directions and magnitudes of magnetic moments on atoms has proven to be more promising. An MCE-based treatment, where parameters of the model are derived directly from *ab-initio* calculations, is able to predict, at quantitative level of accuracy, the magnetic properties of Fe-Cr alloys in a broad range of temperature and Cr concentration, for example the temperature-dependent atomic moments and the Curie temperature. The model does not explicitly treat atomic vibrations, but the inclusion of experimental phonon spectra makes it possible to fully describe the free energies of both the low temperature bcc α-phase and the high temperature γ-phase of the alloy, and to predict the occurrence of the α-γ and γ-α phase transitions in the low Cr concentration range as a function of temperature.

Tools for large scale atomic simulations

The development of molecular dynamics simulations requires accurate parameterization of interatomic interaction laws. The formation of magnetic moments on atoms in iron and iron-based alloys contributes to cohesive energy of the material and therefore has to be included in the treatment of the interatomic forces. In DFT calculations this is taken into account through the exchange-correlation terms, but these terms are neglected in conventional empirical molecular dynamics simulations. Since DFT calculations can only be performed for relatively small systems containing up to ~500 atoms, magnetic potential was developed as means for including electron exchange-correlation effects in the treatment of larger scale multi-million atom simulations. The treatment has now been applied to cascade simulations,

and simulations of extended defects, where for the first time it appears possible to investigate magnetic properties of radiation defects and dislocations.

For Fe-Cr alloys the treatment of interatomic interactions has led to the development of the two-band potential, which is based on the analysis of electronic effects associated with *s*- and *d*-bands. Extensive atomistic simulations performed using the two-band Fe-Cr potential showed that Cr atoms slow down migration of radiation defects in the alloy, and form bound complexes with clusters of self-interstitial defects. Also, application of the two–band potential to the interpretation of experimentally observed resistivity recovery curves explained the origin of the unusual shift of temperatures of the first and the second resistivity recovery stages, where the temperature of stage I decreases whereas the temperature of stage II increases as a function of chromium concentration. Furthermore, the two-band potential predicted the tendency of Cr atoms to segregate to the core of small self-interstitial dislocation loops, in agreement with electron microscope observations.

An outstanding question impeding reliable estimates of defect production in iron and iron alloys was associated with broad scatter in the predicted equilibrium configurations of defects and defect clusters formed in collision cascades. Special effort devoted to the resolution of the problem resulted in the development of several interatomic potentials which, although based on different physical assumptions, were sufficiently in agreement with DFT calculations on the structure and formation energies of point defects. A systematic study of defect production performed using the new generation of potentials improved *by an order of magnitude* the scatter in the predicted number of defects formed in a cascade for a given energy of a primary knock-on atom. An important conclusion derived from these studies is that the presence of chromium does not have any noticeable effect on the production of defects in collision cascades.

Molecular dynamics simulations describing the propagation of edge dislocations through iron containing helium bubbles also showed a systematic trend where helium bubbles, characterized by the relatively low helium to vacancy ratio, were shown not to represent strong obstacles to the propagation of dislocations. The “near-critical” helium bubbles containing near threshold number of helium atoms, on the other hand, were able to strongly affect the propagation of dislocations. Simulations showed a particularly significant role played by the screw dislocation segments formed near a He bubble. The very low mobility of these screw dislocation segments makes the formation of these segments the rate limiting stage controlling the overall rate of mechanical deformation of a material containing pressurized helium bubbles.

Furthermore, using large scale atomistic simulations, significant new information was gained about the interaction of ½<111> dislocations with ½<111> and <100> dislocation loops that contribute to radiation hardening and embrittlement of bcc metals, steels and alloys. The mobility and core structure of segments formed in the corresponding dislocation-dislocation reactions were determined by simulations where various dislocation and loop configurations were considered to assess the obstacle strength associated with both types of the loops. Effects of absorption and transformation of dislocation loops (i.e. change of their Burgers vectors) found in simulations is likely to be responsible for changes in microstructure (loop population) observed experimentally in plastically deformed irradiated Fe and Fe-Cr alloys. Simulations show that the ½<111> dislocation loops represent stronger obstacles for propagating ½<111> edge dislocations than the <100> type loops.

Fundamentals of mechanical deformation and microstructural evolution

Linear and planar defects such as dislocations and grain-boundaries are important elements of microstructure as they act as sinks for radiation defects. Movement and resulting rearrangement of dislocations controls plasticity and fracture behaviour of materials. In He-pre-implanted conventional 9%Cr steels, prior austenitic grain-boundaries have been shown to act as nucleation sites for He-bubbles at high temperatures. At low temperature ~250°C He-pre-implanted ferritic/martensitic steels exhibit lack of ductility with inter-granular failure along the prior austenite grain-boundaries, even if no bubbles are observed by transmission electron microscopy (TEM).

DFT calculations of formation and cohesive energies of selected tilt-boundaries with different excess volumes have been carried out for α-Fe. Comparison with simulations based on empirical potentials showed good agreement for the formation energy of several grain boundaries investigated in the study. The empirical potential-based predictions underestimated by approximately 30% the formation energy of crystal surfaces. The accuracy of predictions made using semi-empirical potentials was worse for the case of grain boundaries, where the difference between these predictions and the DFT values exceeded 40%.

DFT calculations were also applied to the assessment of binding energy between He and grain-boundaries, and the effect of segregated He atoms on the cohesive energy of the grain-boundaries. Due to many-body interaction effects between atoms of the metal, He atoms in substitutional configuration have the highest binding energy if they are located in the *second* nearest layer of atoms with respect of the centre of a grain boundary. Calculations performed using semi-empirical potentials agree well with these DFT predictions. For He in the interstitial position, the binding energy calculated using the presently available empirical potentials does not reproduce the results obtained by DFT calculation, neither quantitatively nor in the form of trends. The DFT-calculated loss of cohesive energy of grain-boundaries due to the presence of He is significantly higher than that calculated for O in Mo, or for P in α-Fe grain-boundaries, which are materials known as those exhibiting significant inter-granular embrittlement effects in the presence of oxygen and phosphorus.

To parameterize kinetic models for He and dpa accumulation in the presence of grain-boundaries, DFT calculations were also conducted for identifying and quantifying the diffusion mechanisms for He along grain-boundaries, and for comparing them to the bulk mechanisms. The activation energy for migration is higher for He diffusion along grain-boundaries than in the bulk, making He diffusion along grain-boundaries slower than in the bulk. Diffusion of He perpendicular to the interface has even higher activation energy. These calculations show also that small He-vacancy clusters are less stable near grain-boundaries than in the bulk. This last conclusion implies the occurrence of a new mechanism for nucleation of helium bubbles at grain boundaries.

Screw dislocations control plastic deformation at relatively low temperatures. The core structure of screw dislocations in bcc transition metals, and their energetics is still a matter of debate. Several configurations of dislocations, minimising image forces and taking into account the boundary conditions, have been investigated using approaches based on Lattice Green's function boundary conditions and the quadrupole arrangement that is most appropriate for adequately treating dislocation in a small cell (~500 atoms). DFT calculations show that dislocation cores are definitively non-degenerate. The energy barrier for the dislocation to move as a whole (the Peierls barrier) was determined, and showed unusual disagreement with results obtained using the most accurate available interatomic potentials. Methodology for calculating, via DFT, the Peierls stress and the double kink formation energies has now been fully developed.

In α-Fe irradiated at high temperature, the observed dislocation loops normally have Bürgers vectors of the <100> type, as opposed to the ½<111> loop types observed under low temperature irradiation. In addition, the elastic stiffness constant C' corresponding to the tetragonal shear deformation (Bain transformation) becomes very small at the transus α -> γ. As a result, elastic properties of α-Fe at high temperature are highly anisotropic. Taking this into account and using the experimental temperature-dependent values for elastic constants, the elastic free energies of dislocations with the <100> and ½<111> Bürgers vectors were evaluated. The free energy of an edge dislocation with the Bürgers vector of the <100> type was found to be proportional to the square root of C', and rapidly decreases near the α -> γ transition temperature. Consequently, the <100> dislocation loops become the most stable defects at high temperature. The stress ahead of their pile-ups is also proportional to the square root of C', resulting in the high temperature softening of iron, in agreement with the hardness data showing nearly zero resistance to deformation near the temperature of the α -> γ phase transition.

Experimental validation

Experimental validation has been an essential part of the programme. So far, most of the validation analysis relied on results published in the open literature. Now there is an opportunity to follow a more robust approach where experiments may be designed bearing in mind new knowledge developed as a result of extensive application of models, to verify experimentally predictions made by modelling.

To assist this objective:

- Several Fe-Cr model-alloys of high purity, as well as alloys containing controlled amounts of C or P atoms have been fabricated and delivered to the programme, and will be extensively used for validation.
- JANNUS, the operation of which is started in January 2009, will allow irradiation in dual or triple beam configuration, and either in-situ or post-mortem examination of microstructure resulting from the accumulation of point defects, He and H.

6. General Objectives:

The general objectives for the materials modelling programme stems from what defines an engineering material and its properties. The programme aims at rationalizing and quantifying:

- What affects the local chemical composition of a particular fusion material, and how significant are the changes in the local chemical composition within a given crystal structure, in terms of their effect on engineering properties. To what extent the chemical stability of a material can be ensured through understanding of fundamental mechanisms of atomic transport and phase stability under irradiation.
- What determines the stability of a particular type of microstructures, at atomic and mesoscopic levels, and what are the timescales of evolution of these microstructures. What are the mechanisms driving microstructural changes as a function of temperature, irradiation conditions, and chemical composition. Are there ways of designing microstructures specifically tailored to irradiation environments, for example those which are self-stabilized (through self-organisation) by the combined effect of high temperature and irradiation. How to assess the effect of mass transport by radiation defects on phase changes occurring in radiation environment.
- What controls the thermodynamic stability and dynamics of evolution of microstructure under mechanical load. These involve questions of phase stability of alloys under high pressure and shearing occurring, for example, near radiation defects and dislocation cores, interaction of mobile dislocations with radiation defects, and the questions of stability of microstructure in relation to plasticity of the material.
- What affects the stability and evolution of interfaces in heterogeneous and complex multi-phase materials under the combined effect of irradiation and thermal environments, how sensitive are the properties of interfaces to the chemical environment (presence of helium, hydrogen, other impurities), particularly in relation to the segregation effects.
- The surface effects, which are particularly significant for modelling plasma facing materials. The properties of plasma facing materials are affected by the combined effect of irradiation and incorporation of deuterium, tritium, and helium atoms/ions directly from plasma. Defects generated by irradiation influence the rate of tritium retention in materials, surface sputtering, blistering (micro-fracture), and the resulting dust production, chemical sputtering. Radiation defects also affect diffusive transport of tritium, deuterium and helium through materials, contributing to the overall transport and retention of tritium, deuterium, and helium in a fusion device.
- Effects of corrosion of materials that are in direct contact with coolant or neutron multiplier materials (lead and lithium). Transmutation reactions in structural materials and in neutron multipliers, as well as radiation damage and radiation assisted transport of mass, are among the significant factors that may affect the corrosion resistance and the lifetime of structural components.

7. The Specific Strategic Objectives:

The specific strategic objectives for the programme are necessarily narrowly defined by the available resources and expertise. By dividing the objectives into broad classes of experimentally observed phenomena, we arrive at the list of main topics given below. The structure of the list reflects the multiscale hierarchy of modelling methods from small scale atomistic to meso- and macroscopic scales. Each objective is largely self-contained, and is expected to be addressed in parallel with other objectives.

Cohesion

1. Perform systematic 0K *ab-initio* study of defect configurations in Fe-Cr model alloys. Determine the lowest energy equilibrium configuration for point defects and clusters of defects, screw and edge dislocation structures, and structures of representative grain boundaries. Find energies for saddle-point configurations of migrating defects (including those of self-interstitial defects, clusters of defects, and double kinks on screw dislocations).
2. Investigate, by means of 0K *ab-initio* methods, interaction of defects, dislocations, and grain boundaries with carbon, nitrogen, helium, hydrogen atoms and, where necessary, with other elements, if there is experimental evidence suggesting that those elements affect properties of EUROFER steel. Assess the effect of carbon and nitrogen on stability and saddle point configurations for migration of defects and dislocations. Develop interatomic potentials for the Fe-Cr-C system describing the Fe-Cr heat of mixing, and the energetics of C impurities in iron-chromium alloys and steels.
3. Develop finite-temperature *ab-initio* (or tight-binding) spin-dynamics electronic structure based model for providing a quantitative estimate for the stiffness parameters of iron and Fe-Cr alloys at elevated temperatures. Develop *ab-initio* treatment of phonon-magnon interactions, and investigate changes in the phonon spectra of iron and iron-based alloys at elevated temperatures (500°C and above).
4. Develop *ab-initio* methods for evaluating free energies of defects and dislocations, assess the free energies for formation and migration of defects and dislocations at high temperatures, taking into account phonon and magnon contributions.
5. Assess, by means of 0K *ab-initio* calculations, the structures formed by the main chemical constituents of (unirradiated) EUROFER steel. This includes creating an easily accessible and verified database of crystal structures for Fe-Cr model alloys, α and α' phases on body-centred cubic (bcc) and face-centred cubic (fcc) lattices, as well as the representative structures for Fe-Cr-C, Fe-Cr-N, Fe-Cr-W, Fe-Cr-V, Fe-Cr-Ta, Fe-Cr-O cluster configurations, and ordered phases, related for example to the formation of carbides, martensitic phases, and the σ-phase

Phase Diagram

6. Develop a Monte-Carlo model for the full concentration-temperature dependent equilibrium phase diagram of Fe-Cr alloys, including γ and σ phases. Parameterize the model and find the minimum parameterization for the phase diagram of Fe-Cr alloy. Investigate the transition from ferritic-martensitic steel microstructures to a fully ferritic microstructure with increased chromium composition.
7. Assess the effect of radiation defects on the phase diagram of Fe-Cr alloys; develop a Monte-Carlo treatment for the phase nucleation events, and model growth of α' and σ phase precipitates. Determine how the finite temperature (free energy) effects associated with defects and dislocation cores, as regions of *localized strong elastic deformations*, influence nucleation of new ordered phases (for example α' and σ-phases) under irradiation. Extend the model to the treatment of mesoscale defects and perform Monte-Carlo simulations, explaining the formation of the (a/2)[111] edge loops in Fe at low temperatures, and a[001] edge loops at high temperatures.
8. Develop a time-dependent spin-polarized Molecular Dynamics model for iron, and extend it to Fe-Cr alloys. Parameterize the model and ensure its consistency with the

equilibrium phase diagram in the low and the high temperature limits. Develop a time-dependent model describing the dynamics of the α-γ phase transformation, the dynamics of formation of α' and σ-phase precipitates.

Collision Cascades

9. Examine the development of collision cascades and radiation damage evolution based on the time-dependent spin-polarized models, in particular the role of spin polarization on damage production, clustering of defects, and the onset of dislocation migration. Assess the effect of phonon-magnon coupling, as well as the effect of carbon on the development of collision cascades, and the subsequent damage production. Assess the effect of the fcc γ-loop on defect production in collision cascades in iron in the limit of high temperature of cascade environment. Describe generation of defects in collision cascades in the α-phase at temperatures close to the α-γ phase transition, taking into account the spin-fluctuation-induced soft phonon modes. Compare with experiments on ion irradiation.
10. Develop a multiscale model for cascade annealing and defect evolution based on a combination of Molecular Dynamics and kinetic Monte-Carlo. Compare with *in-situ* electron microscope observations.

Helium, Hydrogen and Damage Accumulation

11. Develop a quantitative kinetic Monte-Carlo model for migration of He in Fe and Fe-Cr alloys. Achieve quantitative agreement with He desorption experiments in the low and high temperature limits. Explain the origin of the observed rapid increase of He desorption rate above 500°C. Model interaction of He with grain boundaries and dislocations and evaluate the range of binding energies characterising the diffusion of helium in the microstructure of deformed iron, Fe-Cr alloys and steels. Develop a model describing the helium grain boundary embrittlement effect.
12. Develop a quantitative model for migration of He *and hydrogen* near surfaces in iron, Fe-Cr alloys, and tungsten. Describe the observed ion implantation profiles, defect accumulation profiles, and the evolution of these profiles as a function of temperature, time, and irradiation dose rate. Explain the combined synergetic effects of triple beam ion irradiation on swelling, and on other properties of the material.
13. Develop a quantitative model for swelling and voidage of α-Fe, Fe-Cr and EUROFER, including the effect of helium and hydrogen on swelling. Explain the absence of void lattices in iron and vanadium.

Kinetics

14. Develop a model for atomic transport in irradiated concentrated alloys, based on ab-initio and Monte-Carlo, or mean-field, approximations. Assess the timescales for phase decomposition of alloys, compare predictions with experimental observations on ion implanted materials, including the dose rate effects.
15. Investigate, by means of 0K *ab-initio* methods, the effect of self-interstitial atom defects and dislocations on the phase stability of Fe-Cr alloy, and on the stability of martensite phases. Determine if the defects and dislocation cores, as regions of *localized strong elastic deformations*, could act as stable nuclei for new ordered phases (for example α and σ-phases) under irradiation. Explain the formation of α' and σ phases under irradiation in the regions of the concentration-temperature phase diagram where those phases are *not* expected to form according to the equilibrium, *or* mean-field non-equilibrium, argument.
16. Develop a model, based on a combination of the 0K *ab-initio* data and Monte-Carlo and mean-filed simulation methods, for defect migration and agglomeration at *low* temperatures (<300°C) in Fe-Cr alloys under irradiation. Find a method for including the specific "defect shape" and anisotropic elastic signature effects, and the 1D vs 3D defect mobility effects, in kinetic Monte-Carlo simulations. Model migration of mesoscale defects, prismatic dislocation loops, mesoscopic vacancy clusters. Assess

the effect of trapping of defects by carbon, nitrogen and solute atoms on the kinetics of phase transformations. Extend the model to the treatment of interaction of defects with dislocations and grain boundaries. Describe radiation-induced segregation effects near grain boundaries in polycrystalline and nano-crystalline materials, including the dose rate effects.

17. Develop large-scale long-time object Monte-Carlo and mean-field model for microstructural evolution of *ion-irradiated* Fe-Cr model alloys, which includes the treatment of surface effects. Validate the model and achieve quantitative agreement with experiment for a broad range of variation of experimental parameters: dose, dose rate, temperature, concentration of solute atoms in the alloy. Develop a Monte-Carlo model for *in-situ* electron microscope observations of migration of dislocation loops. Identify the type of impurities responsible for the observed pinning of defects.
18. Develop a *deformable-lattice* Monte-Carlo model for Fe-Cr alloys and steels in the high temperature limit close to the α-γ instability temperature (~500°C and above) in the absence of irradiation. Simulate carbon diffusion at high temperatures, the process of formation of martensite, and investigate the dynamics of the α-γ phase transformation. Compare with *in-situ* electron microscope observations of the α-γ phase transformation.

Plasticity and Fracture

19. Develop a fully anisotropic discrete dislocation dynamics (DDD) model for α-Fe and Fe-Cr alloys valid for the temperature range where bcc α phase retains its structural stability. Simulate temperature-dependent plastic yield and tensile properties of pure iron and Fe-Cr alloys. Compare predictions with *in-situ* electron microscopy traction experiments.
20. Develop a linked discrete dislocation dynamics (DDD) – kinetic discrete lattice Monte-Carlo (kMC) approach to the treatment of dislocation climb. Describe the dynamics of formation of jogs on dislocation lines under irradiation, the growth of hexagonal and square shaped dislocation loops, and investigate the role of lattice discreteness effects on dislocation mobility laws. Describe dislocation and defect mobility laws for ordered compounds and alloys, where propagation of defects and dislocations interferes with local chemical order.
21. Derive dislocation mobility laws for bcc metals, iron, iron-chromium alloys and steels, particularly those for screw and mixed dislocations, using Molecular Dynamics and other atomistic methods for modelling deformations at realistic *low* strain rates for conservative (thermally activated glide) and non-conservative (climb) motion of dislocations, in the presence of irradiation defects. Investigate interaction of dislocations with clusters of defects, small dislocation loops, and assess the effect of α' and σ phase precipitates, and the presence of carbon and nitrogen solute atoms on dislocation mobility. Using discrete dislocation dynamics, model irradiation hardening effects in the low and high temperature limit. Identify and quantify the origin of plastic softening of iron, Fe-Cr alloys and EUROFER in the high temperature limit. Identify the part played by grain boundaries versus the dislocation density effects.
22. Develop a model for brittle fracture of pure iron, and extend it to other bcc metals, including Fe-Cr alloys. Develop a model for brittle fracture of *irradiated* iron, other bcc metals, and Fe-Cr alloys. Describe interaction of dislocations with radiation defects, impurities and transmutation products (helium, hydrogen), and identify the origin of DBTT increase. Explain the DBTT saturation effect observed in the limit of low helium transmutation rate. Combine with the study of phase stability, and assess the potential of high temperature operation for minimizing the radiation embrittlement effect. Explain why DBTT recovers if irradiation is performed at elevated temperatures close to or above 400°C in the absence of He production.
23. Extend the treatment to oxide-dispersion strengthened (ODS) steels, and explain the observed increase in strength, and reduction in the fracture properties of ODS steels. Identify the part played by grain boundary effects versus dislocation density effects in strengthening of ODS steels in comparison with non-ODS steels.

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24. Develop a dislocation-based model for thermal creep of iron, model alloys, and EUROFER steel. Assess the accuracy of the model and the relative contribution of various types of dislocations, their interaction with obstacles, and the role of grain size. Explain the effect of oxide dispersion on the suppression of thermal creep.
25. Develop a dislocation-based model for *radiation* creep, treating the combined effect of radiation and temperature, and assessing the range of validity of the Stress Induced Preferential Absorption (SIPA) model, as well as the part played by grain boundaries. Explain the observed weak sensitivity of radiation creep to the presence of obstacles in the material. Assess ways of suppressing radiation creep and the combined effects of thermal and radiation creep.

8. Experimental Validation

As we noted in the Introduction, the objectives that the modelling programme is expected to achieve in the form of new mathematical models and computer programs, should lead to *quantitative* predictions that must be validated and tested experimentally. By comparing predictions with experimental observations one can identify and eliminate errors and incorrect assumptions involved in a particular model or a concept. We expect that every task on materials modelling (listed above in the Specific Objectives section) will have to involve, and should be assessed by means of quantitative comparison with appropriately designed and executed validation experiments.

Predictions are expected to be validated against ion irradiation experiments, where microstructural features observed experimentally should be described, at sufficient level of accuracy, by mathematical models containing no or few adjustable parameters. Microstructural examination should involve electron microscopy and spectroscopy, atom probe microscopy, small angle neutron scattering, and other microscopic and spectroscopic means for experimental examination of materials, and meso- and micromechanical tests performed at suitable spatial and time-scales. Also, the modelling programme should maintain strong links with experimental work on neutron irradiation where models are expected to be validated using simplified binary or ternary alloy systems, as well as realistic materials, including steels and technological alloys and composites, subjected to irradiation in nuclear reactors

9. The Innovative Development of Materials

Understanding the fundamental physical mechanisms controlling in-service properties is a powerful source for knowledge-based development of innovative fusion materials.

The previous programme has clearly established the connection of yield behaviour with the elasticity properties and the phase stability, particularly for the case of the α -> γ phase transformation. Avoiding the occurrence of this transformation and reducing the effect of embrittlement due to α/α' decomposition, or even the σ phase formation at high Cr concentrations, is an obvious challenge that emerges from this investigation. Adding α-promoting chemical elements, which suppress α/α' decomposition and/or the formation of the σ-phase, opens a possible route to developing structural materials with better high temperature strength and radiation stability.

A similar approach should be followed in the development of tungsten based alloys for high temperature applications. Here the transfer of expertise accumulated as a result of extensive investigation of bcc lattice Fe-Cr alloys to tungsten based alloys, and possible extension of work to ternary alloys, is an avenue where modelling methods can be efficiently applied to assist and possibly even guide experimental tests.

10. Conclusion: Implementation and Monitoring

This document gives a comprehensive description of the main objectives to be achieved in the five to seven years to develop reliable modelling tools, based on appropriate physical treatment on the scale, where it can be clearly described and expressed in mathematical terms with the minimum of approximations, and validated using appropriate experiments.

It is the impressive progress made during the preceding period 2003-2008, which allows the present definition of strategic objectives. They are ambitious, requiring development of new modelling tools, which have proven necessary by the new knowledge accumulated during the preceding period of time. In order to progress in achieving these new strategic objectives on the 2010-2015 timescale, the tasks of the MAT-REMEV research project will be selected and evolved with time via a common and continuous scientific assessment conducted every six months, as it was effectively done so far.

A*ssuming at least constant resources*, one can envisage that by 2015, significant progress will be made in the understanding and predictive modelling of microstructure and mechanical properties of Fe-Cr-C model-alloys with significant insight into the EUROFER behaviour. This means that, beyond 2015, modelling should turn progressively more from EUROFER to other materials such as W-alloys, ODS, or completely new materials. Understanding and predicting radiation effects in EUROFER and other materials under DEMO conditions will certainly be advanced enough by 2020 to contribute to the materials science and physical modelling knowledge-based definition of the IFMIF materials test matrix.

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