WP3: Transferability of ion and neutron irradiation

The main goals of this WP are:

- To understand better how the microstructure evolves under irradiation, the mechanisms and factors influencing this evolution, focusing in particular on their effect on ion-neutron-transferability;

- To provide information on the microstructure evolution as well as irradiated samples as input to WP5 and WP6, where the influence of the irradiation-induced microstructure on the deformation behaviour and the mechanical properties as well as characterization-method-related ion-neutron-transferability issues will be addressed.

- To provide guidance to the experiments based on ion irradiation as neutron irradiation surrogate in terms of identification of suitable irradiation conditions and recommendations for PIE, in order to avoid potential ion irradiation specific artifacts.

In the period between Months 18 and 36 the main objectives of this WP were:

1. To take to sufficient maturity the microstructure evolution models based on the OKMC method, in order to be able to apply them to simulate ion irradiation cases of practical interest for the project and compare the results with ion irradiation experiments;

2. Collect the physical parameters that are needed for the models to function, based on literature, experience and partly also work performed in WP2, specifically task 2.1;

3. Benchmark the different codes to ensure consistency when using equivalent parameters.

4. Perform the bespoke ion irradiations that were identified as necessary to study specifically the problem of the artifacts of ion irradiation and the portability of results from ions to neutrons.

5. Start the post-irradiation examination of the ion irradiated specimens.

This WP includes three milestones, and four deliverables. All milestones have been reached as well as two deliverables. Below, a description of the work performed under the different tasks is given.

Task 3.1 Primary damage distribution in ion irradiated and neutron irradiated Fe/FeCr T*ask leader: C. Ortiz, CIEMAT. Other partners – UA*

This task assessed theoretically the best conditions for ion irradiation experiments, to be as close as possible to neutron irradiation in terms of initial damage distribution. **CIEMAT** performed simulations to obtain the recoil energy distribution for fission and fusion neutrons under different configurations, as well as the PKA spectra for protons and Fe ions. Results were compared in terms of defect clustering for both vacancies and self-interstitials. For the case of Fe ion irradiation, the implantation depth profiles were obtained to evaluate the optimal depth for damage characterization. These calculations showed that irradiation with Fe at energies of 5-8 MeV result in clustered fractions that are similar to those expected under neutron irradiation, while the clustered fraction is much lower when using proton irradiation. All these results have been described in detail in the first deliverable of this task: D3.1. *Primary damage distributions in Fe and FeCr* (CIEMAT, UA) *Main author: C. Ortiz, CIEMAT.*

Task 3.2 Advanced nanostructure models for ion- and neutron irradiation conditions.
Task leader: M. J. Caturla, UA. Other partners – CIEMAT, SCK•CEN

The objective of this task is to develop models of damage accumulation in irradiated Fe and FeCr that can be contrasted against the experiments performed in this WP, as well as with the existing neutron experimental data. The simulation tool that has been selected for this task is Object kinetic Monte Carlo (OKMC).

During this period we have focused on two aspects:

(1) Development of the OKMC codes selected to be used in this project. Each code will focus on different aspects of what needs to be modeled as explained below.

(2) Gather all the information available in the literature needed as input parameters for the simulations of Fe and FeCr alloys, including carbon. A parametrization was selected for the simulations to be performed in this task and those parameters that are lacking have been identified.

The developments on each code and tasks performed by each partner are described below. Three codes have been selected, shown schematically in figure 1: (a) Mega-OKMC, developed by CIEMAT (b) MATEO, developed by SCK-CEN and (c) MMonCa, a code developed initially at IMDEA Materials and now being extended by UA.

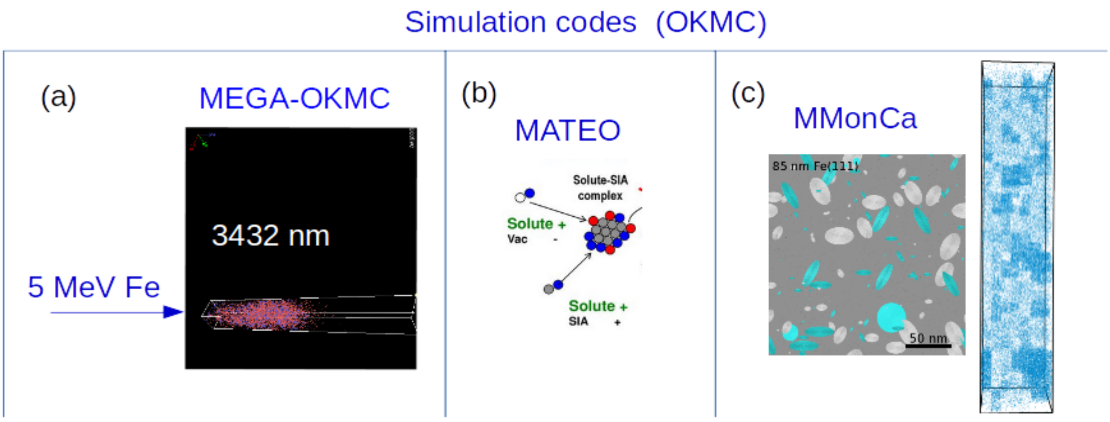

***Figure 1:** OKMC codes used in the project (a) Mega-OKMC (b) MATEO (c) MMonCa*

MEGA-OkMC (Microstructure Evolution GPU-Accelerated) is a code that was recently developed at CIEMAT. It is based on GPU programming and is thus computationally efficient. The parallel algorithm it is based on tries to find the most appropriate time step according to the defects that are present in the simulation box, which allows using time steps order of magnitude larger and thereby, strongly reduces the number of computational steps necessary to reach a given physical time. In particular, it is not limited in space and thus can follow the evolution of defects in large simulation boxes. This is very useful to simulate the evolution of defects in materials irradiated with energetic ions that reach large depths, such as those performed in the framework of M4F. Fig. 2(a) shows the implantation profile corresponding to an implantation of 5 MeV Fe in Fe simulated by MARLOWE code. Note that this is one of the energies used in the irradiations performed under task 3.3. As we can see, ions penetrate up to large depths, about 2 microns. Preliminary simulations were performed with the MEGA code to determine an optimum simulation box in these conditions, as shown in Fig. 2(b) and (c), where defects in boxes of 2.28 and 3.43 microns are shown, respectively. Preliminary results showed that a simulation box of 2.28 microns represents a good compromise between size and computational efficiency. In addition, simulations have been performed for an Fe matrix with different carbon concentrations and the effect of pulsed vs. continuous irradiation has been explored.

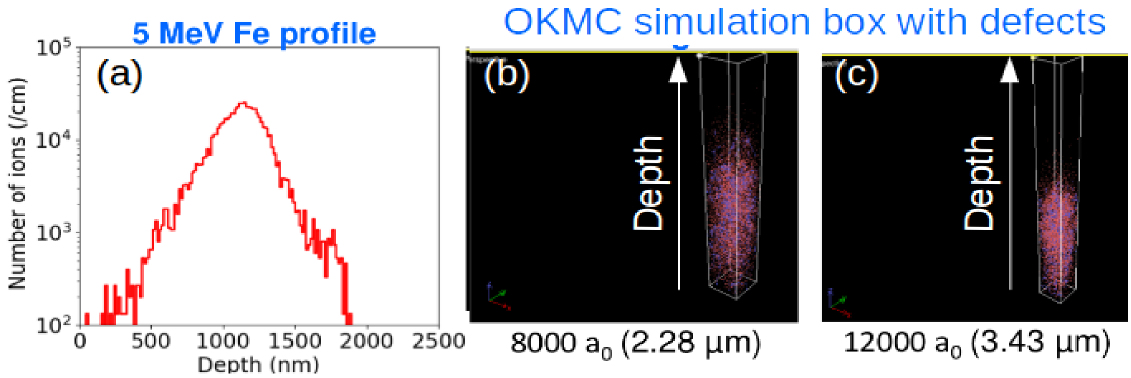

Figure 2: *(a) Depth profile of implanted 5 MeV Fe in Fe as obtained by Marlowe. Mega-OKMC simulation cell with a depth of (b) 2.28 mm and (c) 3.43 mm showing the location of the damage produced by the irradiation.*

A second OKMC code in this WP is MATEO, code being developed by **SCK•CEN.** This code has the capability of modeling the nucleation and evolution of solute rich clusters. In the case of FeCr with the presence of impurities such as Si, Ni or P, or a combination of these, such as those used in the experiments being performed in this project, it is important to be able to model the formation of these clusters. Due to the detail description of these processes, and the fact that it is CPU-based differently from Mega-OKMC, this OKMC code is not able to simulate large system sizes. Nevertheless, the information obtained from these calculations could be transferred to the other OKMC codes in an effective model for solute clustering. The effects of solutes such as Si, Cu, Ni, Mn or P is being studied and results can be compared to experimental results obtained with APT, for example.

The third OKMC code is MMonCa, that was originally developed at IMDEA-Materials in Madrid, and that is currently being extended for the purposes of this project at the **UA**. This code has been developed to include two features: on one hand it includes long range elastic interactions between loops and on the other hand it can model segregation and precipitation of the alloy element induced by point defects. In this period work focused on improving the model for migration of the alloy element by defects introducing the possibility of forming a vacancy-Cr pair or a self-interstitial-Cr pair. Most of the work has been devoted to vacancy-Cr. Using this description, temperature dependence of transport coefficients match those obtained with other, more accurate methods, particularly for the vacancy-drag ratio. The model has been applied to study aging at different temperatures and results have been compared to experimental measurements as well as other simulation methods.

Task 3.3 Ion irradiation to address ion-irradiation-specific transferability issues
Task leader: C. Heintze, HZDR. Other partners – NCBJ

This task is dedicated to the ion irradiation of the different selected samples and conditions. During the first part of the project, the samples and irradiation conditions were selected. During this period all irradiations were performed. Below we include a brief description of the achievements of each partner in this task.

HZDR performed the ion irradiation experiments. Briefly, materials with two different Cr contents have been irradiated, Fe9Cr and Fe14Cr, and with different impurities, P, Si and Ni as well as Eurofer97. Most of the irradiation was of 8 MeV Fe ions although 5 MeV Fe implantation was also performed for some cases. Temperature was kept at 300ºC in all irradiations. Two different fluences and fluxes were used and the effect of a rastered beam vs. a defocused beam was studied. These set of experiments should shed some light in the influence on microstructure evolution of:

- Ion flux
- Ion fluence
- Ion energy
- Rastered focused beam vs. defocussed beam.
- Alloy concentration.
- Impurities and synergy between impurities and alloy elements.

It should be noted that HZDR made a significant effort to address an important issue in ion irradiation of Fe and FeCr alloys: carbon contamination. Specific irradiations as well as analysis using Rutherford backscattering (RBS) and nuclear reaction analysis (NRA) were performed. These experiments revealed a minor C contamination, with most of the effects close to the surface.

NCBJ has performed ion irradiation experiments as a service for WP6. Materials were provided by HZDR and were Fe, Fe9Cr, Fe-9Cr-NiSiSP and Eurofer97. All irradiations were of 275 keV Fe ions. Three different temperatures (room temperature, 300ºC and 450ºC) were used, as well as different doses, from 0.1 dpa up to 10 dpa.

Task 3.4 PIE on irradiated samples using TEM, APT, PAS
Task leader: C. Pareige, CNRS. Other partners – HZDR, CIEMAT

All irradiated samples were delivered to the different partners for their characterization by different methods. Two main tools are being used for this purpose: transmission electron microscopy (TEM) and atom probe tomography (APT).

APT work was performed at CNRS. Figure 3 shows an example of the results being obtained. In this case, Cr rich clusters (red) and NiSiPCr clusters (blue) can be identified and compared for different irradiation conditions: two different energies (8 MeV and 5 MeV) and defocused vs. rastered beam. Preliminary results seem to indicate that beam focusing and rastering does not have a significant effect in Cr cluster concentration or size and a small influence in solute rich clusters (SRC) with lower Ni and Si enrichment for defocused beam and slight number density reduction and similar size. Flux, on the other hand, seems to have an important contribution, with an increase in the number density of Cr-rich clusters for lower flux, while maintaining the same size, and a decrease in number density and an increase in size for SRC for low flux. Note, however, that the irradiation energy was also different which could also have an influence. Another interesting study performed by CNRS is the synergy between different impurities, Si, Ni and P together with C in the formation of SRC.

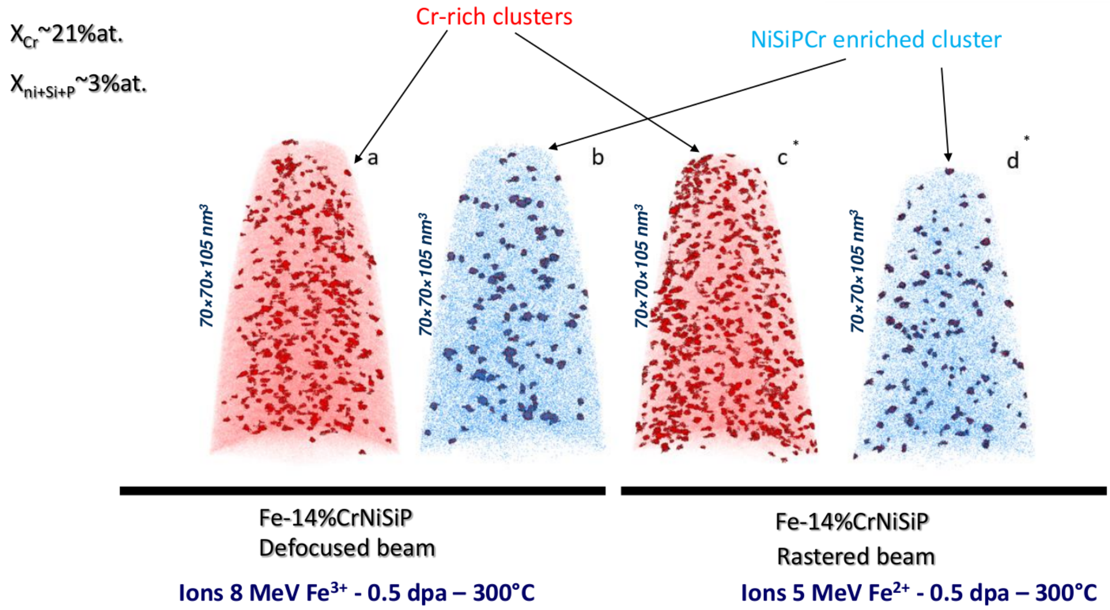

Figure 3: *APT results for two different irradiation conditions: (left) 8 MeV Fe and defocused beam (right) 5 MeV Fe and rastered beam.*

Cross-sectional STEM was performed at HZDR to study the depth-dependent distribution of loops in Fe9Cr ion-irradiated at ion energies of 1 and 5 MeV. This work is aimed at supporting nanoindentation tests in WP6, but also contributes to the background of WP3.