WP4: Deformation mechanisms at the grain scale

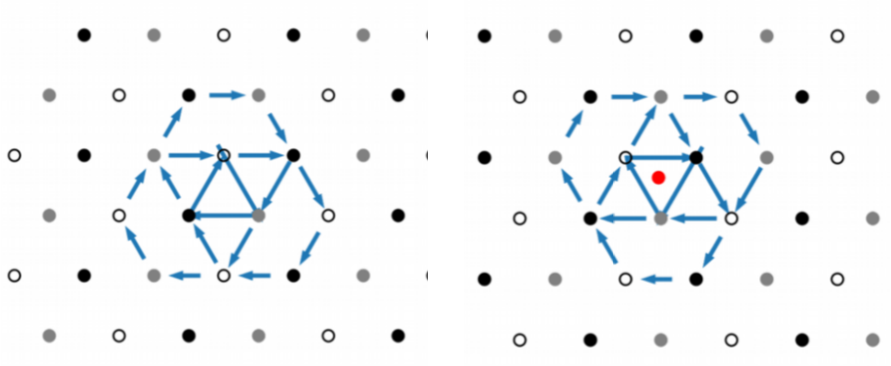
This WP includes four tasks, three devoted to developing models operating at increasingly larger scales and limited experimental content, the fourth one eminently experimental

Task 4.1: Elementary processes of plasticity (M1-M48)
Task leader: D. Rodney, CNRS; other partners: CEA, CIEMAT, SCK-CEN, UPC

This task is subdivided in four sub-tasks: three are devoted to using atomistic models to study the energetic of the interaction between dislocations and solutes/defects, the fourth one compares experimental observations with dislocation dynamic model predictions.

Sub-task 4.1.1: Dislocation mobility law – CNRS (D. Rodney), CEA

In this subtask, it was investigated whether the density functional tight binding (DFTB) method, an approximate density functional theory (DFT) approach, could be used to model dislocations in iron and its alloys. The code dftb+ implementing the DFTB method is freely available at: http://www.dftbplus.org. A new parametrization of DFTB for bulk bcc iron was developed and provided much better elastic constants and lattice parameter, as well as magnetization and electronic band structure. The new parametrization was then used to model the core of a dislocation in pure iron and in presence of carbon interstitials. However, it turns out that, even if DFTB is much less computationally expensive than DFT, this method remains expensive and it is estimated that with the current computational resources, it remains difficult to simulate systems with more than 5,000 atoms, which is not enough to model the full 3D migration process of a dislocation in bulk iron.

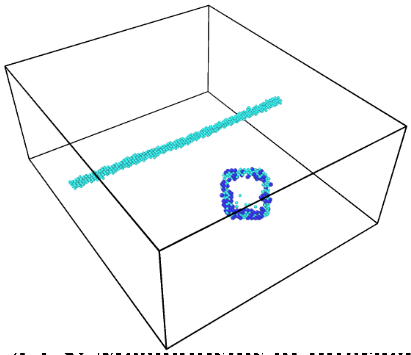


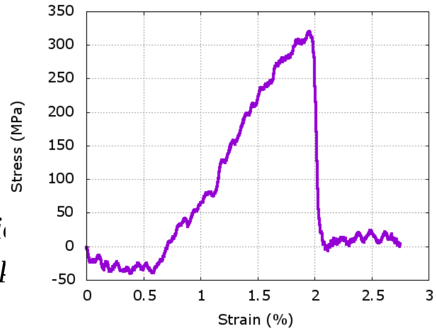
(a) **(b)**

Easy (a) and hard (b) cores relaxed with DFTB in pure iron and in presence of C atoms respectively

Sub-task 4.1.2: Atomic-scale mechanisms of interaction between dislocations and irradiation defects - SCK-CEN (G. Bonny)

The objective of this task is to investigate the combined effect of C and Cr enrichment of loops on the hardening of FeCrC alloys. The atomic scale interaction mechanism between dislocation and CCr decorated loops will be studied. The task is realized in three steps: i) density functional theory (DFT) computations to characterize the interaction between C, Cr and point defects; ii) the development of a ternary FeCrC interatomic potential, fitted to the DFT data; iii) large scale molecular dynamics (MD) simulations employing the interatomic potential to characterize the interaction between a dislocation line and (decorated) loop. The DFT computations are completed and an FeCrC potential compatible with LAMMPS was fitted. Large scale MD simulations using the FeCrC potential are on-going.





Mo … acti … l [100] loop in … rresp

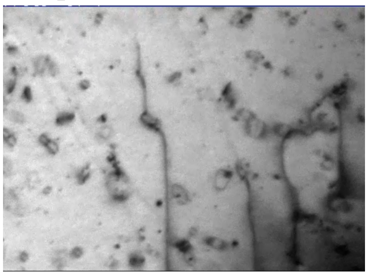
Sub-task 4.1.3: Mechanisms of interactions dislocation-grain boundary to parameterize slip transfer – UPC (N. Anento), CIEMAT, SCK-CEN

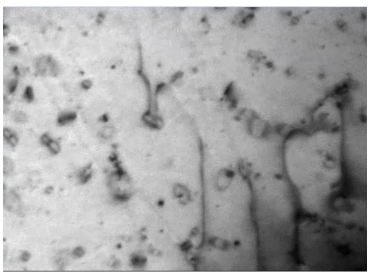
The interaction of dislocations with three different <110> tilt-GBs and a <100> tilt-GB in α-Fe has been investigated by atomistic modelling. The GBs considered have been 1) Σ3(112)<1-10> and vicinal to GB112, 2) Σ11(332)<1-10> and 3) Σ5(310)<100>. Two calculation methods have been used, molecular dynamics (MD) and hybrid continuum-atomistic model.

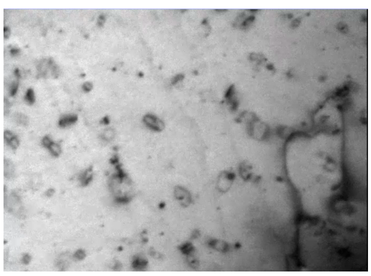
Each GB has been fully characterized establishing all the potential dislocation-GB interactions, for the possible combinations of Burgers vector orientations and dislocation character (edge or mixed). Considering the case of a single dislocation-GB interaction, the only observed outcome at all temperatures is absorption leading to the creation of a GB dislocation (GBD) along with the emission of disconnections. When dislocation pile-up-GB interaction is considered, mainly the reaction observed at all temperatures is also dislocation absorption, although for GB112 we could observe transmission and reflection under specific conditions.

Sub-task 4.1.4: Comparison in-situ TEM/DD simulations to validate the elementary processes of interactions - CIEMAT (M. H. Mayoral), CNRS, CEA

In-situ straining experiments have been started. Both irradiated and pristine samples were prepared by electropolishing for TEM observations. Non-irradiated samples were tested in a wide range of temperature, i.e. between -170°C up to 500°C, in order to investigate the plastic deformation mechanisms at dislocation scale. The observations revealed that at all temperatures dislocations glide in {110} or {112} planes with 1/2[111] Burgers vectors, as expected. The dynamics of dislocations shows that their motion is always jerky. At high temperature, this behavior is exacerbated and culminates with a strong dynamic strain aging at c.a. 400°C, presumably due to the diffusion of interstitial. Below room temperature, dislocations present straight screw segments pinned by super jogs formed by the combination of cross slip and solute pinning. The dislocation mobility has been estimated based on an estimation of the effective stress. Experiments on irradiated samples were carried out at liquid nitrogen temperature where dislocation dynamics is more steady. Several interactions between dislocation loops and mobile screw dislocations were recorded and analyzed. In most cases, irradiation loops are overcome by dislocations after pinning. We highlight the importance of dislocation cross-slip in this process. A close inspection of the loop shape tends to indicate that most of them are restored after interactions, although some others can be pushed along the dislocation line. Further experiments are planned in order to constitute a statistically representative database of interactions. The most suitable examples will be selected for comparison with DD simulations.







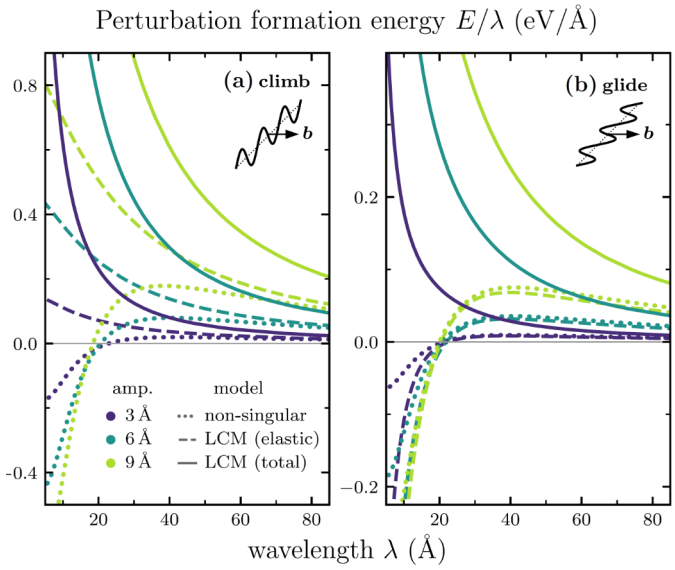
In-situ TEM observation of the interaction between a dislocation and an irradiation loop at T=-170°C.

Task 4.2: Meso-scale study of plasticity (M1-M45)
Task leader: L. Dupuy, CEA; other partners: CNRS, UKAEA

This task is subdivided in two sub-tasks, where the first one is expected to provide input to the second one, together with other subtasks of Task 4.1.

Sub-task 4.2.1: Radiation defect microstructure in the context of dislocation dynamics simulations – UKAEA (S. Dudarev)

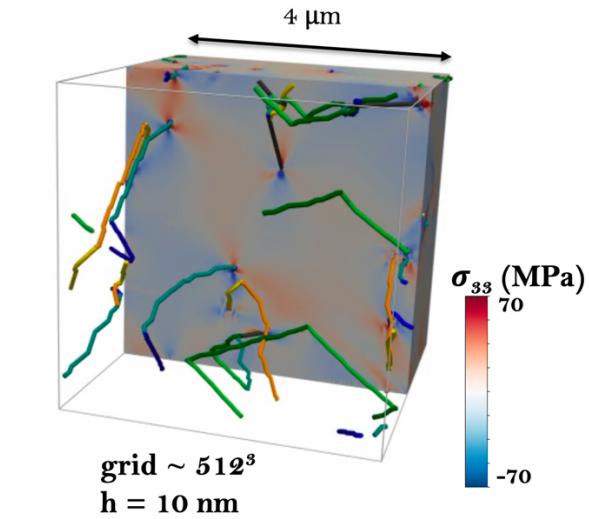
The task was initially formulated in the context of a relatively conventional approach to the treatment of radiation damage, assuming that the microstructure can be classified in terms of some relatively idealized isolated defect objects, for example dislocations, vacancy clusters, dislocation loops etc. The in-depth physical analysis of the problem performed in P.M. Derlet and S.L. Dudarev, Phys. Rev. Mat. **4**, 023605 (2020) showed that the accumulation of radiation defects in steels at temperature below ~300 °C in the high (above 0.1 dpa) dose limit is athermal. Microstructures simulated in the athermal approximation showed that the density of defects and dislocations was high and that the density of vacancies not visible in TEM was also high, in agreement with experimental PAS data. The microstructures are characterized by strongly fluctuating microscopic stresses associated with the defects and they do not exhibit any notable time evolution below ~300°C. Analyzing how such microstructure responds to deformation requires exploring the laws of interaction between dislocations and small-scale defects. The simulations show that the great majority of defects present in the irradiated materials have the size below ~100 Burgers vectors, and hence are in the range where the elastic treatment of dislocation lines exhibits instabilities, see M. Boleininger, T. D. Swinburne, L. Dupuy and S. L. Dudarev, Phys. Rev. Res. **2**, 032033(R) (2020). The effect of instability, which is expected to be compensated by non-linear interactions in the dislocation core, is significant in the context of dislocation dynamics, where the treatment of interaction with small defects is believed to be responsible for the radiation hardening and the strain localization effects. The treatment of dislocations interacting with radiation defects requires evaluating the force acting on a dislocation segment in the presence of point defects, and hence it is necessary to know the stress field generated by these defects. While performing such a calculation appears straightforward, the relevant formulae are not available in literature and need to be derived. Such a derivation has now been performed within the project.



Formation energy of sinusoidal perturbations in (a) climb and (b) glide directions for a 1/2 [111](101) edge dislocation. The nonsingular elasticity theory is compared with the local core model, with (total) and without (elastic) contribution of the core energy. Note the small-wavelength instabilities inherent to the nonsingular theory.

Sub-task 4.2.2: Large-scale simulation of plasticity in irradiated single grains - CEA (L. Dupuy), CNRS

The DD simulation code NUMODIS from CEA was coupled to the elastic solver dedicated to boundary value problems resolution AMITEX_FFTP. Difficulties related to the specific spatial discretization scheme used in code NUMODIS slowed this process down, but are now resolved. Preliminary benchmarks have been performed to assess the accuracy of this elastic solver against a full DD simulation.



Dislocation microstructure and the associated stress field computed using the coupling between microMegas and AMITEX on a 512x512x512 FFT grid.

Task 4.3: Continuum scale modeling of slip localization (M1-M48)
Task leader: I. Simonovski, JRC; other partners: CEA, METU

This task is subdivided in two sub-tasks performed in parallel. The outcome of 4.3.1 will serve to connect the dislocation-based models of WP4 with the coarse-grained models of WP5. Subtask 4.3.2 will predict slip traces to be compared with experimental observations in Subtask 5.4.3.

Sub-task 4.3.1: Continuum modeling of slip localization – JRC (I. Simonovski)

A strain gradient crystal plasticity model has been developed where non-linear hardening equations with non-convex latent hardening laws have been implemented. This model is based on a linear hardening model. Two versions of the non-linear hardening model have been developed: 1) one slip resistance for all three slip systems and 2) each slip system has individual slip resistance. The newly developed models are computationally significantly more demanding than the previous linear hardening model. There are some difficulties with convergence in the very first increment. To alleviate them, two sub-versions have been developed, one with a smooth sign function used in the first increment only and one with the smooth sign function used throughout the whole analysis. This approach improves the convergence but the results are practically the same.

Sub-task 4.3.2: Segment DD computations – CEA (C. Robertson)

Plastic strain spreading in post-irradiated ferritic grains is predicted using a dedicated micro-model developed based on DD simulations accounting for dislocation/defect interactions and cross-slip [K. Gururaj et al., JNM 459 (2015) 194-204]. The model explains how the internal stress landscape evolutions control the dose-dependent development of wavy shear bands, characterized by the «plastic strain spreading ratio», defined as the number of shear bands in irradiated over non-irradiated case and noted N_{irr}/N_{00dpa} ($N_{irr}/N_{00dpa} < 1$ denotes plastic strain localisation). Quantitative N_{irr}/N_{00dpa} evolutions are calculated for various grain size, irradiation defect size D and defect number density n conditions. The conclusions drawn out of this approach are as follows:

1) N_{irr}/N_{00dpa} systematically increases with plastic strain level $\square_p$;

2) N_{irr}/N_{00dpa} sharply decreases with growing defect size D, for any fixed defect number density n and plastic strain level $\square_p$;
3) shear band spacing distribution (i.e. the distribution width and maximum value) depends on the nD product, thus scales with the disperse barrier hardening effect;
4) shear band thickness distribution (i.e. the distribution width and maximum value) also depends on $1/D$ affecting the local, defect-scale dislocation configuration and corresponding internal stress landscape;
5) homogeneous ($N_{irr}/N_{00dpa} \geq 1$) to localized ($N_{irr}/N_{00dpa} < 1$) straining mechanism transition depends on i)-the mutual band-to-band interaction stress intensity, ii)-the internal stress level relative to the defect strength $\square_{defect}$ [T. Nogaret et al., JNM 380 (2008) 22-29].
6) strain localisation is slightly more pronounced for decreasing grain size, for a fixed n and D.

The proposed approach allows finding the dose-dependent elongation limit trends and establishing corresponding strain deformation maps [K. Farrell et al., JNM 335 (2004) 471-486]. The model applicability to poly-crystalline ferritic materials is evaluated using a specific stochastic calculation procedure, based on observations of ion irradiated/deformed grain aggregates (cf. Task 4.4).

Task 4.4: Validation through the experimental study of slip localization (M1-M48)
Task leader: M. H. Mayoral, CIEMAT; other partners: PSI

Proton irradiation of TEM in-situ straining specimens have been performed. Specimens will be shipped to CIEMAT by September 2020. Due to a failure at the microscope at CIEMAT, the possibility to perform the experiments in another facilities, where active material can be handled, and with the suitable sample-holder is explored. These experiments are foreseen to start by early 2021. Regarding experiments at PSI, the irradiation is already done and FIB sample preparation is started.
Materials under study will be G385-Fe9Cr and single crystal Fe-16Cr (99.95%), with (110) oriented surface. In both cases, the proton irradiation conditions are selected to focus on the early stages of dislocation free channel formation: 300 °C as irradiation temperature and 1 dpa. Proton irradiation is performed at 7.2 MeV. A degrader has been employed to get a flat damage profile up to 50 microns in depth.